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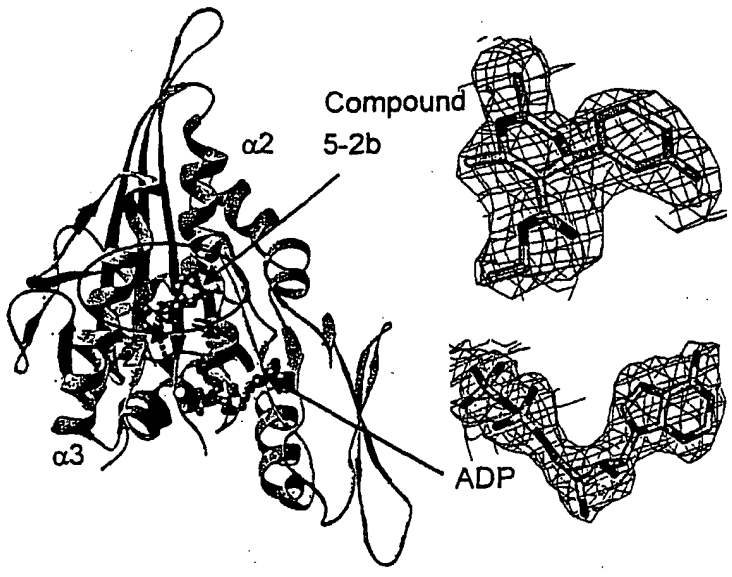
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(54) Title: MITOTIC KINESIN BINDING SITE



(57) Abstract: The present invention is directed to the identification, characterization and three-dimensional structure of a novel ligand binding site of KSP. Binding of ligands to the novel binding site result in a conformational change in the three-dimensional structure of the protein and a modulation of the activity of KSP. This conformational change in turn results in the formation of a novel binding pocket in the KSP protein, which comprises the novel binding site of the instant invention.

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TITLE OF THE INVENTION
MITOTIC KINESIN BINDING SITE

FIELD OF THE INVENTION

The present invention generally pertains to the fields of molecular biology, protein purification, protein crystallization, X-ray diffraction analysis, three-dimensional structural determination, rational drug design and molecular modeling of motor proteins, in particular - Kinesin Spindle Protein (KSP). Compositions and crystals of KSP with a KSP inhibitor bound to the protein at the novel ligand binding site identified herein are also provided. The crystallized KSP is physically analyzed by X-ray diffraction techniques. The resulting X-ray diffraction patterns are of sufficiently high resolution to be useful for determining the three-dimensional structure of inhibitor-bound KSP. Those atomic coordinates are useful in molecular modeling of related proteins and rational drug design (RDD) of mimetics and ligands for KSP and related proteins. Methods of using the structure coordinates of KSP in complex with an inhibitor for the design of pharmaceutical compositions which inhibit the biological function of KSP, particularly those biological functions mediated by molecular interactions involving KSP are also disclosed.

BACKGROUND OF THE INVENTION

Cancer remains one of the leading causes of death in the United States. Clinically, a broad variety of medical approaches, including surgery, radiation therapy and chemotherapeutic drug therapy are currently being used in the treatment of human cancer (see the textbook CANCER: Principles & Practice of Oncology, 6th Edition, De Vita et al., eds., J. B. Lippincott Company, Philadelphia, Pa., 2001). However, it is recognized that such approaches continue to be limited by a fundamental lack of a clear understanding of the precise cellular bases of malignant transformation and neoplastic growth.

The control of cell division is one of the most basic aspects of multicellular existence. Uncontrolled cell growth and division, which produces cells that divide when they should not, produces contiguous cellular masses called tumors that are the basis for many cancers.

A common strategy for cancer therapy is the development of drugs that interrupt the cell cycle during mitosis. Compounds that perturb shortening (depolymerization) or lengthening (polymerization) cause arrest of the cell cycle in mitosis due to perturbation of the normal microtubule dynamics necessary for the chromosome movement. (Compton, D. A., et al., (1999) Science 286:913-914). A common denominator attending these compounds is that they arrest cells in mitosis by inhibiting spindle assembly (Compton, D. A., et al., (1999) Science 286:313-314). More recently, some agents such as monastrol have been implicated in inhibiting mitosis by blocking the function of essential proteins, such as mitotic proteins. (Mayer, T.U. et al., (1999) Science 286: 971-974).

The motor protein, kinesin, was discovered in 1985 in squid axoplasm. R. D. Vale et al., Identification of a Novel Force-generating Protein, Kinesin, Involved in Microtubule-based Motility, *Cell* 42:39-50 (1985). In the last few years, it has been discovered that kinesin is just one member of a very large family of motor proteins. E.g., S. A. Endow, The Emerging Kinesin Family of Microtubule Motor Proteins, 16 Trends Biochem. Sci. 221 (1991); L. S. B. Goldstein, The Kinesin Superfamily: Tails of Functional Redundancy, 1 Trends Cell Biol. 93 (1991); R. J. Stewart et al., Identification and Partial Characterization of Six Members of the Kinesin Superfamily in Drosophila. *Proc. Nat'l Acad. Sci. USA* 88:8470 (1991). Other motor proteins include dynein, e.g. M.-G. Li et al., Drosophila Cytoplasmic Dynein, a Microtubule Motor that is Asymmetrically Localized in the Oocyte, *J. Cell Biol.* 126:1475-1493 (1994), and myosin, e.g. T. Q. P. Uyeda et al., *J. Mol. Biol.* 214:699-710 (1990).

Mitotic kinesins are enzymes essential for assembly and function of the mitotic spindle, but are not generally part of other microtubule structures, such as in nerve processes. These essential microtubule-based motor proteins travel along microtubules reaching into every corner of the cell. Mitotic kinesins play essential roles during all phases of mitosis. These proteins can be conceptualized as biological machines that transduce chemical energy into mechanical forces and motion. Kinesins use the energy derived from ATP hydrolysis to power their movement unidirectionally along microtubules and to transport molecular cargo to specific destinations. During mitosis, kinesins organize

microtubules into the bipolar structure that is the mitotic spindle. Kinesins mediate movement of chromosomes along spindle microtubules, as well as structural changes in the mitotic spindle associated with specific phases of mitosis. Experimental perturbation of mitotic kinesin function causes malformation or dysfunction of the mitotic spindle, frequently resulting in cell cycle arrest and cell death. It is rapidly becoming clear that mictrotubule motors play a crucial role in the functions of microtubules in mitosis.

Among the mitotic kinesins which have been identified is Kinesin Spindle Protein (KSP). KSP belongs to the BimC family of kinesins which are essentially a conserved kinesin subfamily of plus end-directed microtubule motors that assemble into bipolar homotetramers consisting of anti-parallel homodimers. Human KSP (also termed HsEg5) has been described [Blangy, et al., Cell, 83:1159-69 (1995); Whitehead, et al., Arthritis Rheum., 39:1635-42 (1996); Galgio et al., J. Cell Biol., 135:339-414 (1996); Blangy, et al., J Biol. Chem., 272:19418-24 (1997); Blangy, et al., Cell Motil Cytoskeleton, 40:174-82 (1998); Whitehead and Rattner, J. Cell Sci., 111:2551-61 (1998); Kaiser, et al., JBC 274:18925-31 (1999); GenBank accession numbers: X85137, NM004523 and U37426] , and a fragment of the KSP gene (TRIP5) has been described [Lee, et al., Mol Endocrinol., 9:243-54 (1995); GenBank accession number L40372]. Xenopus KSP homologs (Eg5), as well as Drosophila K-LP61 F/KRP 130 have been reported. KSP is a mitotic kinesin protein essential for proper DNA division in cells.

During mitosis KSP associates with microtubules of the mitotic spindle. Microinjection of antibodies directed against KSP into human cells prevents spindle pole separation during prometaphase, giving rise to monopolar spindles and causing mitotic arrest and induction of programmed cell death. The current model of KSP function in mitosis envisions that KSP and related kinesins in other, non-human organisms, bundle antiparallel microtubules and slide them relative to one another, thus forcing the two spindle poles apart. KSP may also mediate anaphase B spindle elongation and focussing of microtubules at the spindle pole. The mitotic spindle has been the subject of considerable research. The study of mitotic spindle proteins, such as microtubules, has yielded anti-mitotic compounds with important applications in cancer chemotherapy. The

demonstrated effectiveness of these anti-mitotic compounds in important medical and agricultural applications demonstrates the desirability of identifying and characterizing anti-mitotic compound development candidates.

Because defects in the function of KSP have been implicated in cell cycle arrest, agents and/or compounds that modulate the activity of this kinesin will find use in the treatment of hyper-proliferative cell disorders such as cancer.

Medicaments generally exhibit their biological activities through strong interactions with their respective targets. Recently, advances in protein crystallography and computational chemistry have introduced a new method of structure-based drug design into the field of drug development. X-ray crystallography (crystallography) is an established, well-studied technique that provides what can be best described as a three-dimensional picture of what a molecule looks like in a crystal. Scientists have used crystallography to solve the crystal structures for many biologically important molecules. Many classes of biomolecules can be studied by crystallography, including, but not limited to, proteins, DNA, RNA and viruses.

Crystallography has been used extensively to view ligand-protein complexes for structure-based drug design. To view such complexes, known ligands are usually soaked into the target molecule crystal, followed by crystallography of the complex. Sometimes, it is necessary to co-crystallize the ligands with the target molecule to obtain a suitable crystal.

Given a "picture" of a target biomolecule or a ligand-protein complex, scientists can look for pockets or receptors where biological activity can take place. Thereafter, scientists can experimentally or computationally design high-affinity ligands (or drugs) for the protein/receptors. Computational methods have alternatively been used to screen for the binding of small molecules. This approach is also useful for developing new anti-mitotic agents.

Recently, independent efforts have confirmed the role of mitotic kinesins as critical mediators of microtubule organization during mitosis. It is postulated that blocking the biological function of motor proteins, e.g., human KSP, will lead to cell cycle arrest. While the binary

structure of KSP complexed with ADP has been published, (Turner et al., Journal of Biological Chemistry, 276; 25496-25502 (2001), no ternary structure of KSP complexed with a modulator, e.g., inhibitor, has heretofore been published. Consequently, until the present invention, which details the structural coordinates of human KSP with various ligands, albeit inhibitors, the identity and characterization of the novel binding site detailed herein was heretofore never available for rational drug design. As such, drug discovery efforts directed towards the KSP protein have been hampered by the lack of structural information about this protein and its complex with a ligand, e.g., monastrol. Such structural information would provide valuable information in discovery of anti-mitotic agents.

The inventors provide herein crystals of KSP, complexed with a ligand, containing a novel, induced-fit binding site and have determined its three-dimensional structure. With this information, it is now possible, for the first time, to rationally design inhibitors of KSP, which can function as anti-mitotic agents, e.g. compounds which inhibit spindle pole separation during mitosis, thereby effectively inducing cell cycle arrest. It is believed that no one has heretofore reported determining the three-dimensional structure of the binding site identified herein.

Advantageous therapeutic embodiments would therefore comprise therapeutic and/or diagnostic agents based on or derived from the three-dimensional crystal structure of KSP including its novel binding site identified herein that have one or more than one of the functional activities of KSP. Additional therapeutic embodiments would comprise therapeutic and/or diagnostic agents based on or derived from molecular modeling of other members of the BimC protein family using the three-dimensional crystal structure of KSP and its binding site provided herein.

In accordance therewith, the novel-binding site disclosed herein is considered a potential target for anti-mitotic agents. In addition, the invention provides a process for creation of ligand candidate structures by means of a computer, using the structural coordinates of KSP's binding site provided herein. Furthermore, the information provided herein will enable one to search for ligand structures from a three-dimensional structure database containing known compounds.

SUMMARY OF THE INVENTION

The present invention is directed to the identification, characterization and three-dimensional structure of a novel ligand binding site of KSP. Binding of ligands to the novel binding site result in a conformational change in the three-dimensional structure of the protein and a modulation of the activity of KSP. This conformational change in turn results in the formation of a novel binding pocket in the KSP protein, which comprises the novel binding site of the instant invention. It has been further discovered that the formation of the novel binding pocket is facilitated by the concurrent binding of a nucleotide substrate or substrates to the protein. Moreover, the instant invention provides an attractive target for the rational design of potent and selective inhibitors of KSP identified by the methods of the invention, particularly new lead compounds useful in treating hyper-proliferative and KSP-dependent disorders.

BRIEF DESCRIPTION OF THE DRAWINGS

FIGURE 1 An X-ray oscillation diffraction picture from a crystal of KSP in complex with (+)-monastrol and ADP (Compound 5-2b).

FIGURE 2 The KSP-ADP-(+)-monastrol complex as shown in a ribbon presentation. The structure of the KSP-ADP-(+)-monastrol (Compound 5-2b) complex is shown in a ribbon representation. The bound conformations of ADP and Compound 5-2b are also given together with their respective electron density. The location of Compound 5-2b, the active isomer of monastrol, is seen at a novel induced-fit site, some 12Å distal from the nucleotide-binding site and catalytic center of the enzyme.

FIGURE 3 (+)-Monastrol binding between helix-α2 and helix-α3. (+)-monastrol (Compound 5-2b) is seen to bind in between (the insertion loop of) helix-α2 and helix-α3 (which is immediately preceding the 'Switch 1' typically seen in all kinesins). Also shown are the side-chains of Arg119, Tyr211 and Trp127. The Arg119 and Tyr211 residues move upward and outward, yielding space to accommodate the binding of the

inhibitor. At the same time, the insertion loop of helix-α2 relocates its main-chain location with a downward shift of ~8Å; the side-chain of its Trp127 as a result swings inward by ~10Å, capping the entrance of the induced-fit cavity together with the side-chains of Arg119 and Tyr211. Lining the newly formed pocket and surrounding the inhibitor are residues 115–119, 127, 130, 132–134, 136, 137, 160, 211, 214, 215, 217, 218, 221 and 239.

FIGURE 4 Comparison between the binary and ternary structure shown in ribbon presentation. The conformational alteration observed for the kinesin structure upon Compound 5-2b binding to the ADP-binary complex is not limited to the immediate vicinity of the inhibitor. Rearrangements of protein moieties are spread throughout the enzyme upon (+)-monastrol binding, including the switch I, switch II and neck linker region, with the exception that the nucleotide binding site of the protein as well as its β-sheet structure remaining basically unchanged.

FIGURE 5 Conformational alteration of KSP structure upon ligand binding shown in ribbon presentation. In the Switch I area of KSP, as circled, the main-chain re-orients its geometry significantly on both ends of Ala230. Although the helicity of the Switch I region is unchanged, the pitch at the C-terminal end of helix-α3 is increased in the ternary complex from that in the binary complex.

FIGURE 6 Conformational alteration of KSP structure upon ligand binding shown in ribbon presentation. In the Switch II region of KSP, which is located on the opposite side of the binding site, as circled, the C-terminal end of helix-α-4 is repositioned significantly. The tip of the helix, in the Switch II region of KSP, near Arg305 is moved by ~6Å in the ternary complex from its location in the binary complex.

FIGURE 7 Conformational alteration of KSP structure upon ligand binding shown in ribbon presentation. In the neck-linker region of KSP, which is the C-terminal portion of the protein construct, the residues

beginning from Lys357 to Phe362 swing by almost 180° in the ternary complex from its position in the ADP binary complex. Although residues 363–368 are present in the protein, they are disordered in the crystal and hence offer no electron density. The neck-linker region of KSP is circled. A close-up view is depicted, comparing the neck-linker region in the ternary complex to that in the binary complex.

FIGURE 8 Conformational alteration of KSP structure upon ligand binding. A close-up view comparing the nucleotide-binding site in the binary and ternary complexes of KSP is shown. Within experimental errors, most of the backbone and side-chains for the two complexes in this region of the protein can be super-positioned.

FIGURE 9 Motor Domain of Human KSP, Amino Acids 1-368.

FIGURE 10 Binding Pocket of human KSP.

FIGURE 11 KSP/Compound 5-2b fluorescence data. Compound 5-2b demonstrates a dose dependent decrease on the fluorescence of Trp127 in the presence of ADP or AMPPNP. These data indicate that the fluorescence assay is useful to measure potential KSP inhibitors. In the absence of the nucleotide, 5-2b does not cause a decrease on Trp127 fluorescence, suggesting the inability of 5-2b to bind to KSP in the absence of the nucleotide.

FIGURE 12 KSP/Compound 8-1 fluorescence data. Compound 8-1 demonstrates a dose dependent decrease on the fluorescence of Trp127 in the presence of ADP or AMPPNP. These data indicate that the fluorescence assay is useful to measure potential KSP inhibitors. In the absence of the nucleotide, 8-1 does not cause a decrease on Trp127 fluorescence, suggesting the inability of 8-1 to bind to KSP in the absence of the nucleotide.

FIGURE 13 KSP/Compound 1-7 fluorescence data. Compound 1-7 demonstrates a dose dependent decrease on the fluorescence of Trp127 in the presence of ADP or AMPPNP. These data indicate that the fluorescence assay is useful to measure potential KSP inhibitors. In the absence of the nucleotide, 1-7 does not cause a decrease on Trp127 fluorescence, suggesting the inability of 1-7 to bind to KSP in the absence of the nucleotide.

FIGURES 14A and 14B KSP Inhibitor Pharmacophore Models. The two pharmacophore models derived from analysis and further computational processing of the crystallized complex are illustrated. Spheres represent a center of a hydrophobic group and boxes represent either a hydrogen bond acceptor (HA) or hydrogen bond donor (HD). All distances are in Å.

FIGURE 15 KSP Inhibitor Pharmacophore Models in KSP Binding Site. A schematic view of the two pharmacophore models superimposed and mapped onto the ligand binding site of KSP defined, in part, by the amino acids of Figure 10. Only relevant KSP protein residues are shown.

FIGURE 16 KSP Inhibitor Pharmacophore Model. A pharmacophore model derived from analysis and further computational processing of a crystallized complex is illustrated. Spheres represent a center of a hydrophobic group and boxes represent either a hydrogen bond acceptor (HA).

TABLE 1 KSP motor domain/Compound 5-2b X-ray coordinates.

TABLE 2 KSP motor domain/Compound 1-7 X-ray coordinates.

TABLE 3 KSP motor domain/Compound 2-7 X-ray coordinates.

TABLE 4 KSP motor domain/Compound 4-2a X-ray coordinates.

TABLE 5 Novel KSP ligand binding site/Compound 5-2b X-ray coordinates.

DETAILED DESCRIPTION OF THE INVENTION

"Conservative substitutions" are those amino acid substitutions which are functionally equivalent to the substituted amino acid residue, either by way of having similar polarity, steric arrangement, or by belonging to the same class as the substituted residue (e.g., hydrophobic, acidic or basic), and includes substitutions having an inconsequential effect on the three-dimensional structure of KSP with respect to the use of said structure for the identification and design of KSP or KSP complex inhibitors, for molecular replacement analyses and/or for homology modeling.

Amino acid sequence "similarity" is a measure of the degree to which aligned amino acid sequences possess identical amino acids or conservative amino acid substitutions at corresponding positions.

A "fragment" of KSP is meant to refer to a protein molecule which contains a portion of the complete amino acid sequence of the wild type or reference protein.

As used herein, a "variant" of a KSP protein refers to a polypeptide having an amino acid sequence with one or more amino acid substitutions, insertions, and/or deletions compared to the sequence of the invention receptor protein. Generally, differences are limited so that the sequences of the reference (native or wild type KSP) and the variant are closely similar overall, and in many regions, identical. Such variants are generally biologically active and necessarily have less than 100% sequence identity with the polypeptide of interest.

Preferably, the biologically active variant KSP has an amino acid sequence sharing at least about 80% amino acid sequence identity with the reference KSP, preferably at least about 85%, more preferably at least about 90%, and most preferably at least about 95%. Amino-acid substitutions are preferably substitutions of single amino-acid residues. Preferably, such polypeptides also possess characteristic structural features and biological activity of a native KSP polypeptide.

For example, variants of KSP are characterized as containing key functional residues that participate in ligand binding. These polypeptide fragments, in turn, have been derivatized by methods akin to traditional drug development. Preferred polypeptides and polynucleotides of the present invention are expected to have, *inter alia*, similar biological functions/properties to their homologous polypeptides and polynucleotides. Furthermore, preferred polypeptides and polynucleotides of the present invention have at least one GPR25 activity.

Sequence similarity or percent similarity can be determined, for example, by comparing sequence information using sequence analysis software such as the GAP computer program, version 6.0, available from the University of Wisconsin Genetics Computer Group (UWGCG). The GAP program utilizes the alignment method of Needleman and Wunsch (J. Mol. Biol. 48:443, 1970), as revised by Smith and Waterman (Adv. Appl. Math. 2:482, 1981).

As used herein, a "binding site" refers to a region of a molecule or molecular complex that, as a result of its shape and charge potential, favorably interacts or associates with another agent (including, without limitation, a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound, antibody or drug) via various covalent and/or non-covalent binding forces.

The terms "ligand binding site" and "binding site" are used interchangeably and refer to a region of a human KSP resulting from the complex of a ligand with KSP. It is believed that this ligand binding site, as a result of its shape and charge potential, favorably interacts or associates with a ligand or binding partner, which is preferably an inhibitor of KSP function. The binding of the ligand to this binding site induces global conformational changes to the KSP protein, thereby potentially modulating the mitotic activity of the protein and thereby inhibiting cell division and facilitating cell cycle arrest. A ligand binding site according to the present invention may include, for example, the actual site of any one of the herein disclosed compounds binding with KSP, as well as any other moiety - chemical or biological - which preferably inhibits the activities of KSP by binding to the ligand binding site disclosed herein.

As used herein, the terms "bind" and "binding" when used to describe the interaction of a ligand with a binding site or a group of amino acids means that the binding site or group of amino acids are capable of forming a covalent or non-covalent bond or bonds with the ligand.

Preferably, the binding between the ligand and the binding site or amino acid(s) is non-covalent. Such a non-covalent bond includes a hydrogen bond, an electrostatic bond, a van der Waals bond or the like. The binding of the ligand to the binding site may also be characterized by the ability of the ligand to co-crystallize with KSP within the novel binding pocket of the instant invention. It is further understood that the use of the terms "bind" and "binding" when referring to the interaction of a ligand with the novel binding site of the instant invention includes the covalent or non-covalent interactions of the ligand with all or some of the amino acid residues comprising the binding site.

A "KSP complex" refers to a co-complex of a molecule/complex comprising the KSP in bound association with a ligand either by covalent or non-covalent binding forces at the binding site disclosed herein. A non-limiting example of a KSP complex includes KSP-(+)-monastrol, or KSP bound to any one of the compounds listed herein.

The present invention relates to the three-dimensional structure of ligand bound-KSP or of a KSP analogue, and more specifically, to the structure of KSP's binding site as determined using X-ray crystallography and various computer modeling techniques. The coordinates of KSP bound to ADP and one of the ligand compounds described herein as shown in Tables 1-4 (relating to the entire motor domain), are useful for a number of applications, including, but not limited to, the characterization of a three-dimensional structure of KSP including its novel binding site, as well as the visualization, identification and characterization of a KSP ligand binding site. The ligand binding site structure(s) may then be used to predict the orientation and binding affinity of a designed or selected inhibitor of KSP, a KSP analogue or of a KSP complex. In general, KSP structures referred to herein are the KSP–ligand bound conformation of KSP. As an example, when referring to an antibody specific for the KSP of the invention, it means an antibody having an affinity for the KSP-ligand bound conformation disclosed herein.

In particular, the invention is drawn to the three-dimensional structure of a ligand bound KSP e.g., when bound to a ligand, preferably an inhibitor.

The amino acid sequence of the motor domain of human KSP is depicted in SEQ ID NO:1. These amino acids correspond to residues 1-368 of the native protein. Another aspect of the invention is a substantially pure isolated amino acid of the amino acid sequence set forth in SEQ ID NO:1. Another aspect of the invention is a variant of that isolated amino acid. Preferably the variant of the amino acid of SEQ ID NO:1 comprises one or more amino acid substitution(s) or deletion(s) of one or more of the amino acids that form the novel binding pocket of the instant invention. More preferably the variant of the amino acid of SEQ ID NO:1 comprises an amino acid substitution of one of the amino acids which form the novel binding pocket of the instant invention.

Another aspect of the invention is an isolated variant of KSP wherein the variant comprises one or more amino acid substitution(s) or deletion(s) of one or more of the amino acids that form the novel binding pocket of the instant invention. More preferably the variant of KSP comprises an amino acid substitution of one of the amino acids which form the novel binding pocket of the instant invention.

The KSP of the invention preferably comprises a ligand binding site characterized by the amino acid residues as set forth in Figure 10 or the relative structural coordinates of those amino acid residues according to Tables 1-4 ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2.0 Å (or more preferably, not more than about 1.0 Å, and most preferably, not more than about 0.5 Å). It is understood that the amino acids listed above represent the residues defining the novel binding pocket formed upon the complexation of a ligand of the invention with KSP. It is further understood that specific binding interactions between the listed residues may or may not occur based on the size of the ligand and structure of the ligand. It is also understood that the computational length of the allowable van der Waals interactions is also a factor when determining whether an amino acid residue binds to a ligand. It is therefore understood that the binding of a ligand of the instant invention may take place between those residues listed in Figure 10 or a subset thereof.

It has been surprisingly discovered that compounds previously disclosed as kinesin inhibitors, and other recently identified

inhibitors of KSP, bind to the KSP protein at the novel binding site described herein. In particular, (+)-monastrol (Compound 5-2b), a compound previously described as inhibiting KSP kinesin activity (see Mayer, T. U. et al. Science 286:971 (1999)) has been found to be a ligand of the novel binding site of the invention. Inhibitors of KSP have also been disclosed in pending U.S. provisional applications Ser. Nos. 60/344,453 (Case 20990PV), 60/338,383 (Case 20995PV), 60/338,380 (Case 20996PV), 60/338,779 (Case 20997PV), 60/338,344 (Case 20998PV), 60/338,379 (Case 20999PV), 60/362,922 (Case 21047PV), 60/383,449 (Case 21018PV), 60/383,478 (Case 21060PV), 60/388,621 (Case 21114PV, filed June 14, 2002) and 60/388,828 (Case 21119PV, filed June 14, 2002). Additionally, inhibitors of KSP kinesin activity are described in PCT Publications WO 01/30768 and WO 01/98278.

The 3-dimensional structure of KSP, bound with Mg^{++}-ADP and Compound 5-2b, was determined at 2.5Å resolution. Compound 5-2b was found to bind to KSP via an induced-fit some 12Å away from the catalytic center of the enzyme, resulting in the creation of a previously unknown binding pocket that is non-existent in the absence of Compound 5-2b (or the other ligands described herein). The binding of Compound 5-2b also introduced significant alteration to the structural conformation in other regions of the KSP motor protein, with the interesting exception that the nucleotide-binding pocket was virtually unaltered from that seen in the ADP binary complex. An analysis of the temperature-factor distribution in the ADP binary and ADP/5-2b ternary complexes of KSP revealed that the protein region surrounding the induced-fit binding pocket of 5-2b became highly rigid upon 5-2b binding.

Using the seeding method, high quality single crystals were obtained for KSP prepared in the presence of ADP and 5-2b. A diffraction data set to 2.5Å resolution was collected and processed in the orthorhombic $P2_12_12_1$ space group. The R_{sym} was 0.084 and the data completeness was 99%. The cell dimensions were 69.5Å, 79.5Å and 159.0Å. An oscillation X-ray diffraction picture of a KSP crystal is given in Figure 1.

The 3-dimensional, tertiary structure of KSP, bound with Mg^{++}-ADP and 5-2b, was determined at 2.5Å resolution with use of phases derived from a combination of molecular replacement, extensive manual

rebuilding, and dynamic refinement. Two identical protein complexes were found in the asymmetric unit of the crystal and were related by a local, non-crystallographic 2-fold axis. For each, the electron density of the protein as well as those of the ligands (ADP, Mg^{++}, and 5-2b) was all well defined. 5-2b was seen to be of the S handedness. Residues 2–17, 272–286, and 363–368 were disordered and showed no electron densities (The N-terminal Met1 residue was processed upon expression).

The structure of the KSP/ADP/Compound 5-2b complex is shown (Figure 2) in a ribbon representation. The bound conformations of ADP and 5-2b are also given together with their respective electron density. The location of 5-2b is seen at a novel induced-fit site, some 12Å distal from the nucleotide-binding site and catalytic center of the enzyme. An enlarged section of this region is shown in Figure 3, together with 5-2b.

In Figure 3 the Compound 5-2b is seen to bind in between (the insertion loop of) helix-α2 and helix-α3 (which is immediately preceding the 'Switch 1' typically seen in all kinesins). Also shown are the side-chains of Arg119, Tyr211 and Trp127. The Arg119 and Tyr211 residues move upward and outward, yielding space to accommodate the binding of the inhibitor. At the same time, the insertion loop of helix-α2 relocates its main-chain location with a downward shift of ~8Å; the side-chain of its Trp127 as a result swings inward by ~10Å, capping the entrance of the induced-fit cavity together with the side-chains of Arg119 and Tyr211. Lining the newly formed pocket and surrounding the inhibitor are the amino acid residues listed in Figure 10. A comparison of this region in the binary and ternary complex is given in Figure 4.

The binding pocket of Compound 5-2b is novel and not previously known, insofar that this binding site does not exist until an inhibitor binds. Hence, this pocket is "induced-fit" by a ligand such as Compound 5-2b. This allosteric binding pocket, located away from the nucleotide-binding site of the motor protein, is not restricted to Compound 5-2b, but is also observed upon the crystal structure determination of complexes of KSP with other compounds of diverse chemical structure that are inhibitors of KSP activity. These results have a profound impact on the design of non-active-site directing inhibitors of KSP.

In a further embodiment of the invention is a method of causing a conformational alteration in the structure of KSP by exposing the KSP to a ligand of the novel ligand binding site of the instant invention. The conformational alteration observed for the kinesin structure upon Compound 5-2b binding (and the binding of other compounds) to the ADP-KSP binary complex is not limited to the immediate vicinity of the inhibitor. Rearrangements of protein moieties are spread throughout the enzyme upon 5-2b binding, with the exception that the nucleotide binding site of the protein as well as its β-sheet structure remain basically unchanged. Among the changes away from the induced-fit pocket, three are noteworthy:

1. In the Switch I area of KSP, as circled in Figure 5 and in a close-up view, the main-chain re-orients its geometry significantly on both ends of Ala230. It can be seen that although the helicity of the Switch I region is unchanged, the pitch at the C-terminal end of helix-α3 is increased in the ternary complex from that in the binary complex.

2. In the Switch II region of KSP, which is located on the opposite side of the 5-2b binding site as circled in Figure 6 and in a close-up view, the C-terminal end of helix-α4 is repositioned significantly. The tip of this helix near Arg305 is moved by ~6Å in the ternary complex from its location in the binary complex.

3. In the neck-linker region of KSP, which is the C-terminal portion of our protein construct, the residues beginning from Lys357 to Phe362 swing by almost 180° in the ternary complex from its position in the ADP binary complex. Although residues 363–368 are present in our protein, they are disordered in the crystal and hence offer no electron density. The neck-linker region of KSP is circled in Figure 7. A close-up view is depicted comparing this region in the ternary complex to that in the binary complex.

In addition to these changes, there are other smaller regional repositionings of main-chains and side-chains of the protein. Most interestingly, the nucleotide-binding site of the motor protein, where ATP hydrolysis occurs, is basically unaltered upon 5-2b binding. A close-up view comparing this site in the binary and ternary complexes of KSP is shown in Figure 8. Within experimental errors, most of the backbone and

side-chains for the two complexes in this region of the protein can be super-imposed.

The effect of overall conformational changes induced by Compound 5-2b could also be examined by comparing the distribution of temperature factors.

High quality single crystals were also obtained for other compounds that are inhibitors of KSP. 3-Dimensional structure determined at 2.5 Å with those crystals demonstrated that the other inhibitor compounds also induce-fit into the protein in the same manner as compound 5-2b.

Consequently, an embodiment of the invention provides protein crystals of KSP complexed with a ligand bound to the ligand binding site disclosed herein and methods for making KSP or a KSP homolog. The crystals provide means to obtain atomic modeling information of the specific amino acids and their atoms forming the binding site and that interact with molecules e.g., ligands or binding partners that bind to the KSP, via the binding site.

The crystals also provide modeling information regarding the protein-ligand interaction, as well as the structure of ligands bound thereto. The KSP crystal or a KSP homolog according to the present invention can be obtained by crystallizing it with a material or compound or molecule which binds to the herein disclosed binding site of the KSP. The KSP crystal according to the present invention includes KSP (human Eg5) and the material which binds to the specific binding site of KSP.

Preferred crystalline compositions of this invention are capable of diffracting X-rays to a resolution of better than about 3.5 Å, and more preferably to a resolution of about 2.6 Å or better, and even more preferably to a resolution of about 2.0 Å or better, and are useful for determining the three-dimensional structure of the material. (The smaller the number of angstroms, the better the resolution.)

The relative structural coordinates of the amino acid residues of the KSP motor domain, when the X-ray diffraction is obtained for the crystalline complex of KSP and a ligand compound described herein, are shown in Tables 1-4.

In another aspect, the present invention provides the three-dimensional structure of human KSP as well as the identification and

characterization of a binding site there within. The identification of this site permits design and identification of compounds that bind to the ligand binding site and modulate KSP related activities. The compounds include inhibitors which specifically inhibit cell proliferation.

Of equal import is the fact that knowledge of the three-dimensional structure of the binding site of KSP provides a means for investigating the mechanism of action of the protein and tools for identifying inhibitors of its function.

As used herein, a ligand binding site also includes KSP or KSP analog residues which exhibit observable NMR perturbations in the presence of a binding ligand, such as any one of the herein disclosed inhibitors or any other ligand. While such residues exhibiting observable NMR perturbations may not necessarily be in direct contact with or immediately proximate to ligand binding residues, they may be critical to KSP residues for rational drug design protocols.

For example, knowledge of the three-dimensional structure of the ligand binding site allows one to design molecules, preferably pharmaceutical agents, capable of binding thereto, including molecules which are thereby capable of inhibiting the interaction of KSP with its native ligands, thereby inducing cell arrest.

Assays may be performed and the results analyzed to determine whether the agent is an inhibitor (i.e., the agent may reduce or prevent binding affinity between KSP and its native ligand/binding partner), or has no effect on the interaction between KSP and its native ligand. Agents identified using the foregoing methods, and preferably inhibitors of KSP, may then be tested as therapeutics in the treatment and/or prevention of hyper-proliferative cell disorders and other diseases that are also characterized by the presence of the hyper-proliferative cells such as cancer.

Once a KSP binding agent/inhibitor has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its selectivity and binding properties – that is its affinity for the ligand binding site disclosed herein. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. Such substituted chemical compounds may then be analyzed for efficiency of fit the ligand binding site of KSP by the same computer methods described in detail above.

Various molecular analysis and rational drug design techniques are further disclosed in U.S. Pat. Nos. 5,834,228, 5,939,528 and 5,865,116, as well as in PCT Application No. PCT/US98/16879, published as WO 99/09148, the contents of which are hereby incorporated by reference.

In another aspect of the instant invention, the high quality single crystals of the KSP complexes comprising the KSP, ADP and the compounds described herein could be used to obtain single crystals of a KSP complex which comprises a compound that weakly binds to KSP or one or more weakly binding fragments of a compound that binds to KSP. This method may be termed intra-crystal ligand exchange. Thus, for example and not limiting in the scope of this embodiment, high quality single crystals of KSP-ADP-Compound 5-2b complex are exposed to the crystallization buffer described in the Materials and Methods which further contains 1mM of a test compound that weakly binds to KSP. It is expected that the test compound will intercalate into the crystal and replace the compound 5-2b in the binding site. One or more molecular fragments of compounds that strongly bind to KSP may also be utilized in this technique.

X-ray diffraction data may be collected (as described in the Materials and Methods) from the high quality single crystals obtained by the intra-crystal ligand exchange technique. The 3-dimensional, tertiary structure of KSP bound to such a weakly binding compound could be utilized to guide the structural modification of the compound and, as a result, optimize the binding of the modified compound to KSP. The 3-dimensional tertiary structure of KSP bound to molecular fragment(s) could be utilized to guide in the identification of a new template for a compound having optimal binding to KSP.

Once the material is designed or selected, the affinity of the material to KSP may be calculated. For the inhibitor to be effective, it should have a high affinity for the ligand binding site, low energy difference between that energy calculated before and after binding. The affinity of the inhibitor may be measured by calculating the dissociation constant of the complex of KSP and the inhibitor. The dissociation constant is preferably 100 micromoles or less. The inhibitor preferably also maintains the bonding with KSP stably after binding. In order to do this, electrostatic repulsion such as charge-charge interactions, dipole-dipole and charge-dipole interactions between the inhibitor and KSP should not occur or be minimized. The sum of electrostatic interaction should be neutral or give a positive effect to the enthalpy of the bonding. Examples of programs designed for calculating such affinity include, but

are not limited to as follows: Gaussian 92, revision C [M. J. Frisch, Gaussian, Inc., Pittsburgh, Pa. © 1992]; AMBER, version 4.0 [P. A. Kollman, University of California at San Fransisco, © 1994]; QUANTA/CHARMM [Molecular Simulations, Inc., Burlington, Mass. © 1994]; and Insight II/Discover (Biosysm Technologies Inc., San Diego, Calif., © 1994). Using the lead compound selected by the method, a stronger inhibitor can be made or designed. This process will be described below.

As well, any compound or anti-mitotic agent (lead compound) selected or designed in accordance with the methods disclosed herein can be changed or modified. Atoms, substituents or a part of the structure may be altered to increase the binding affinity to KSP. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It is noted that components known in the art to alter conformation should be avoided. The substituted chemical compounds may then be analyzed for fit with KSP by the same computer methods described herein.

After the material designed by the computer method described above is prepared and bound to KSP to produce a crystal, the 3-dimensional structure of the complex may be determined at high enough resolution (over 0.28 nm) using X-ray crystallographic methods. The information gained therefrom e.g., about the interaction between KSP and the inhibitor obtained from this can then be used to modify the inhibitor and to increase the affinity of the inhibitor for the ligand binding site of KSP.

Thus, for example, those atoms considered to be involved in binding to the ligand binding site of KSP disclosed herein can be mutated by exchanging one or more of the amino acid residues in the ligand binding site or in the motor domain of KSP that eventually effects the function of KSP on the underlying cell. As an example, if a cell's hyper-proliferative state is not effected by the mutated KSP, it may be surmised that the mutation very likely has not affected the function of KSP. In the alternative scenario, where the mutation decreases the hyper-proliferative state of the diseased cell, then one may surmise that the mutation has affected the ability of KSP to function in its intended purpose, e.g. hydrolyze ATP to ADP or bind microtubule etc. due to the substitution of the amino acid residue. This method can be used to identify amino acid residues in the original KSP which are important in the binding of the ligand to the binding site of KSP disclosed herein.

Once the amino acid residues in the ligand binding site of KSP have been identified as involved in the overall function attending KSP, the structure of the binding site can be identified based on the three-dimensional structure of KSP. Based on the structure of the binding site, a compound such as a peptide or other compound can be screened and designed which will fit into the three-dimensional model of the binding site.

Likewise, just as the three-dimensional modeling of KSP is provided by the present invention using the coordinates from the X-ray defraction patterns, these can be either analyzed directly to provide the three-dimensional structure (if of sufficiently high resolution). Alternatively, the atomic coordinates for the crystallized KSP, as provided herein, can be used for structure determination. The X-ray diffraction patterns obtained by methods of the present invention, can be provided on computer readable media, and used to provide electron density maps.

The electron density maps, provided by analysis of the X-ray coordinates of KSP complexed with Compound 5-2b, provided herein, may then be fitted using suitable computer algorithms to generate secondary, tertiary and/or quaternary structures and/or domains of KSP, which structures and/or domains are then used to provide an overall three-dimensional structure, as well as binding and/or active sites of KSP.

Knowledge obtained concerning KSP including the binding site defined herein can also be used to model the tertiary structure of related kinesin proteins, in particular members of the BimC protein family.

As an example, the structure of renin has been modeled using the tertiary structure of endothiapepsin as a starting point for the derivation. Model building of cercarial elastase and tophozoite cysteine protease were each built from known serine and cysteine proteases that have less than 35% sequence identity. The resultant models were used to design inhibitors in the low micromolar range. (Proc. Natl. Acad. Sci. 1993, 90, 3583).

Furthermore, alternative methods of tertiary structure determination that do not rely on X-ray diffraction techniques and thus do not require crystallization of the protein, such as NMR techniques, are simplified if a model of the structure is available for refinement using the additional data gathered by the alternative technique. Thus, knowledge of the tertiary structure of the KSP binding site provides a significant window to the

structure of the other kinesin family members. Thus, an embodiment of this invention envisions use of atomic coordinates of KSP protein, or fragment, analog or variant thereof, to model a KSP protein.

One skilled in the relevant art may use conventional molecular modeling methods to identify a ligand binding site of a KSP of another species. Specifically, coordinates provided by the present invention may be used to characterize a three-dimensional structure of the target KSP molecule, liganded or unliganded. Importantly, such a skilled artisan may, from such a structure, computationally visualize a putative binding site and identify and characterize other features based upon the coordinates provided herein. Such putative ligand binding sites may be further refined using chemical shift perturbations of spectra generated from various and distinct KSP complexes, e.g. from other species, competitive and non-competitive inhibition experiments, and/or by the generation and characterization of KSP or ligand mutants to identify critical residues or characteristics of the ligand binding site.

Such identification of a putative ligand binding site is of great import in rational drug design.

It is noted that in order to use the structural coordinates generated from the complex KSP described herein in Tables 1-4, it may be necessary to display the relevant coordinates as, or convert them to, a three-dimensional shape or graphical representation, or to otherwise manipulate them. In general, such a three-dimensional representation of the structural coordinates will find use in rational drug design, molecular replacement analysis, homology modeling, and mutation analysis. This is typically accomplished using any of a wide variety of commercially available software programs capable of generating three-dimensional graphical representations of molecules or portions thereof from a set of structural coordinates. The scientific art is replete with conventional software programs, which are incorporated by reference herein in their entirety. Refer to, for example, GRID (Oxford University, Oxford, UK); AUTODOCK (Scripps Research Institute, La Jolla, Calif.); Flo99 (Thistlesoft, Morris Township, N.J.) etc.

For storing, transferring and using such programs, a machine, such as a computer, is also contemplated, which produces a three-

dimensional representation of the KSP binding site. The machine would comprise a machine-readable data storage medium comprising a data storage material encoded with machine-readable data. Machine-readable storage media comprising data storage material include conventional computer hard drives, floppy disks, DAT tape, CD-ROM, and other magnetic, magneto-optical, optical, floptical and other media which may be adapted for use with a computer. The machine further comprises a working memory for storing instructions for processing the machine-readable data, as well as a central processing unit (CPU) coupled to the working memory and to the machine-readable data storage medium for the purpose of processing the machine-readable data into the desired three-dimensional representation. As well, the machine of the present invention further comprises a display connected to the CPU so that the three-dimensional representation may be visualized by the user. Accordingly, when used with a machine programmed with instructions for using said data, e.g., a computer loaded with one or more programs of the sort identified above, the machine provided for herein is capable of displaying a graphical three-dimensional representation of the KSP complex described herein and set forth in Tables 1-4.

The structural coordinates of the present invention enable one to use various molecular design and analysis techniques in order to (i) solve the three-dimensional structures of related molecules, preferably molecular complexes such as those of other species or members of BimC family of proteins; as well as (ii) design, select, and synthesize chemical agents capable of favorably associating or interacting with a ligand binding site of a KSP molecule, wherein the molecular chemical entity would preferably inhibit KSP function including inducing mitotic arrest in cells contacted therewith.

Thus, the present invention provides a method for determining the molecular structure of a molecular complex whose structure is unknown, comprising the steps of obtaining the molecular complex whose structure is unknown, e.g., from a related species, and then generating NMR data there from. The NMR data from the molecular complex whose structure is unknown can then be compared to the structure data obtained from the KSP complex of the present invention. Then, 2D, 3D and 4D isotope filtering, editing and triple resonance NMR techniques can be used to conform the 3D structure described

herein for the KSP complexes disclosed in Tables 1-4 to the NMR data from unknown target molecular complex. Alternatively, molecular replacement may be used to conform the 3D structure of the present invention to X-ray diffraction data from crystals of the unknown target molecular complex.

Molecular replacement involves correctly orienting and positioning the known structure into the crystal unit cell of the unknown structure. This is accomplished by a six dimensional (three positional and three rotational) search process that involves computation of a set of theoretical diffraction data using the known structure for every orientation and position searched and comparing it with the observed diffraction data of the unknown structure. The best match defines the correct position and orientation of the known structure in the unknown unit cell. This match offers phase information for use in conjunction with X-ray diffraction data of the unknown structure for the determination of its 3-dimensional structure.

In another aspect, this invention envisions use of atomic coordinates of the KSP protein disclosed herein, to design a chemical compound capable of associating with KSP or a fragment, analog or variant thereof.

For example, one method of this invention for evaluating the ability of a chemical entity to associate with any of the proteins or protein-ligand complexes set forth herein comprises the steps of: a) employing computational means to perform a fitting operation (docking) between the chemical entity and a binding pocket or other surface feature of the molecule or molecular complex; and b) analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket.

In another aspect, the invention envisions use of atomic coordinates of the KSP protein to design a model of ligands in the binding site defined herein.

Preferred embodiments of the aforementioned uses are those wherein the KSP protein comprises a binding site characterized by amino acid residues as set forth in Figure 10.

As a general rule, one may use knowledge of the geography of the various regions of the ligand binding site disclosed herein, e.g. hydrophobic and/or hydrophilic to design KSP analogs (mutant) in which

the overall KSP structure is not changed, but change does affect biological activity ("biological activity" being used here in its broadest sense to denote function). Thus, one may make changes to the amino acid sequences to effectively obtain a KSP analog/mutant that exhibits a greater affinity for its binding ligand. As well, one may correlate biological activity to structure. If the structure is not changed, and the mutation has no effect on biological activity, then the mutation has no biological function. If, however, the structure is not changed and the mutation does affect biological activity, then the residue (or atom) is essential to at least one biological function.

Similar molecular modeling is also provided by the present invention for rational drug design (RDD) of mimetics and ligands of KSP, "ligand" being used in the broadest sense, referring to any substance capable of observable binding to the KSP protein at the herein disclosed binding site. The drug design paradigm uses computer modeling programs to determine potential mimetics and ligands which are expected to interact with sites on the protein. The potential mimetics or ligands are then screened for activity and/or binding. For KSP-related mimetics or ligands, screening methods can be selected from assays for at least one biological activity of KSP, e.g., anti-mitotic activity. Thus, an embodiment of the invention envisions use of the structural information from the ligand/protein complexes found herein including the information derived therefrom in designing new chemical or biological moieties that bind tighter, bind more specifically, have better biological activity or have better safety profile than known ligands that bind KSP.

The computer modeling method disclosed herein can also be used to remodel the mimetics or ligands to improve the affinity or solubility, and produce an optimized pharmaceutical agent.

The resulting optimized mimetics or ligands can thereafter be prepared and the inhibitory activity for KSP can be tested *in vitro* and *in vivo*. If the test confirms that the material does indeed inhibit KSP, then the material or a derivative can be used as an anti-mitotic agent. Using the method as described above, the compound identified to have inhibitory activity may thereafter be used as a lead compound to obtain an improved inhibitor.

In order to confirm the affinity predicted by the computer modeling method, the dissociation constant of the complex may be experimentally measured.

The resulting mimetics or ligands are then provided by methods of the present invention and are useful for treating, inhibiting or preventing KSP-modulated diseases in animals, including humans. Preferably the ligands of the novel binding site provided herein are useful in the treatment or prevention of a hyper-proliferative disease, preferably cancer. Preferably, the ligand(s) identified by the methods described herein are useful in the treatment of cancer.

The ligands identified by the methods of this invention may be administered to mammals, preferably humans, either alone or, preferably, in combination with pharmaceutically acceptable carriers, excipients or diluents, in a pharmaceutical composition, according to standard pharmaceutical practice. The ligands can be administered orally or parenterally, including the intravenous, intramuscular, intraperitoneal, subcutaneous, rectal and topical routes of administration.

As used herein, the term "composition" is intended to encompass a product comprising the specified ingredients in the specific amounts, as well as any product which results, directly or indirectly, from combination of the specific ingredients in the specified amounts.

The pharmaceutical compositions containing the active ingredient may be in a form suitable for oral use, for example, as tablets, troches, lozenges, aqueous or oily suspensions, dispersible powders or granules, emulsions, hard or soft capsules, or syrups or elixirs. When a ligand according to this invention is administered into a human subject, the daily dosage will normally be determined by the prescribing physician with the dosage generally varying according to the age, weight, sex and response of the individual patient, as well as the severity of the patient's symptoms.

In one exemplary application, a suitable amount of a ligand of the novel KSP ligand binding site is administered to a mammal undergoing treatment for cancer. Administration occurs in an amount between about 0.1 mg/kg of body weight to about 60 mg/kg of body weight per day, preferably of between 0.5 mg/kg of body weight to about 40 mg/kg of body weight per day.

Consequently, an object of the invention is to provide a method for determining the three-dimensional structure of a protein containing the ligand binding site as disclosed herein, or a complex of the protein with a ligand thereof, using homology modeling techniques and structural coordinates for a composition of this invention. Homology modeling involves constructing a model of an unknown structure using structural coordinates of one or more related proteins, protein domains and/or subdomains. Homology modeling may be conducted by fitting common or homologous portions of the protein or peptide whose three-dimensional structure is to be solved to the three-dimensional structure of homologous structural elements. Homology modeling can include rebuilding part or all of a three-dimensional structure with replacement of amino acids (or other components) by those of the related structure to be solved.

One of the objects of this invention is to provide three-dimensional structural information on new complexes of BimC family members of which KSP is a member with various ligands, as well as muteins or other variants of any of the foregoing. To that end, the invention provides for the use of the structural coordinates of a crystalline composition of this invention, or portions thereof, to solve, e.g., by molecular replacement, the three-dimensional structure of a crystalline form of such a ligand-protein complex, typically involving a protein containing at least one ligand binding site as disclosed herein. Doing so involves obtaining X-ray diffraction data for crystals of the protein-ligand complex for which one wishes to determine the three-dimensional structure. Then, one determines the three-dimensional structure of that protein or complex by analyzing the X-ray diffraction data using molecular replacement techniques with reference to the previous structural coordinates. As described in U.S. Pat. No. 5,353,236, for instance, molecular replacement uses a molecule having a known structure as a starting point to model the structure of an unknown crystalline sample.

Still further, the invention also includes compositions and methods for identifying binding sites of other members of the BimC protein family. The methods involve examining the surface of a protein of interest, preferably a kinesin, to identify residues that facilitate binding to the binding site. The residues can be identified by homology to the ligand binding site of

human KSP described herein. Overlays and super-positioning with a three-dimensional model of a KSP binding site, or a portion thereof that contains a ligand binding site, also can be used for this purpose.

An alternative method of this invention provides for selecting from a database of chemical structures a compound capable of binding to a BimC family protein. The method starts with structural coordinates of a crystalline composition of the invention, e.g., coordinates defining the three-dimensional structure of a BimC family protein or a portion thereof e.g., the herein provided coordinates relative to human KSP. Points associated with that three-dimensional structure are characterized with respect to the extent of favorable interactions with one or more functional groups. A database of chemical structures is then searched for candidate compounds containing one or more functional groups disposed for favorable interaction with the protein based on the prior characterization. Compounds having structures which best fit the points of favorable interaction with the three-dimensional structure are thus identified.

An exemplary embodiment of the invention provides methods for identifying and designing small molecules that bind to the binding site using atomic models of KSP provided herein. The method involves modeling test compounds that fit spacially into the binding site of interest using an atomic structural model comprising a KSP binding site or portion thereof, screening the test compounds in a biological assay characterized by binding of a test compound to KSP, and identifying a test compound that binds to KSP.

Also provided is a method for identifying a potential inhibitor of KSP, comprising the steps of using a three-dimensional structure of a KSP binding site as defined by the relative structural coordinates set forth in Table 5 or the relative structural coordinates of the amino acids of Figure 10 as set forth in Tables 1-4 to design or select a potential inhibitor, and obtaining or synthesizing said potential inhibitor. The inhibitor may be selected by screening an appropriate database, may be designed de novo by analyzing the steric configurations and charge potentials of an empty KSP binding site in conjunction with the appropriate software programs, or may be designed using characteristics of known inhibitors to create "hybrid" inhibitors. The inhibitor may then be contacted with KSP, and the effect of

the inhibitor on KSP related function may be assessed. For instance, a potential inhibitor identified by this method may be contacted with KSP in the presence of one or two KSP substrates selected from ATP and microtubules, and determining the effect the potential inhibitor has on KSP ATPase activity. It is also within the confines of the present invention that a potential inhibitor may be designed or selected by identifying chemical entities or fragments capable of associating with KSP; and assembling the identified chemical entities or fragments into a single molecule to provide the structure of the potential inhibitor.

In furtherance of the above, there is provided a method for identifying an anti-mitotic agent comprising providing the atomic coordinates comprising the relative atomic structural coordinates of the amino acids of Figure 10 as set forth in Tables 1-4 ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2.00Å thereof to a computerized modeling system; modeling compounds which fit spacially into the KSP binding site; and identifying in an assay for KSP activity a compound that inhibits or decreases the activity of the KSP through binding to the binding site.

Once the agent has been identified, it may be contacted with KSP and the effect the agent has on KSP may then be assessed. In addition, the agent may be contacted with KSP in the presence of a KSP binding molecule and the effect the agent has on binding between KSP and the KSP binding molecule may then be assessed.

Also disclosed herein is a process for identifying a potential anti-mitotic agent which upon binding to a human KSP inhibits cell proliferation, the process comprising the steps of:

a) exposing the KSP to a mixture of at least two potential ligands;

b) attempting to crystallize said KSP in the presence of said mixture;

c) if crystals are obtained, obtaining an X-ray diffraction pattern of the KSP crystal; and

d) determining whether a ligand/KSP complex is formed by comparing the electron density map calculated from the X-ray diffraction pattern of said KSP crystal

when exposed to said mixture of said at least two potential ligands to the electron density map calculated from the X-ray diffraction pattern set forth in a table selected from Table 1, 2, 3 and 4.

Also provided herein is a method of identifying a compound that modulates the binding of a ligand to a ligand binding site of a human KSP, said method comprising: modeling test compounds that fit spatially into a KSP ligand binding site using an atomic structural model of a KSP binding site having the relative structural coordinates as set forth in a table selected from the group consisting of Tables 1, 2, 3 and 4 for the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F), ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å; screening the test compounds in an assay characterized by binding of a ligand to the ligand binding site; and identifying a test compound that modulates binding of said ligand to the KSP at its binding site.

Further provided is a method for identifying a potential inhibitor of human kinesin spindle protein (KSP), the method comprising the steps of :

(i) providing a three-dimensional structure of a ligand-bound KSP as defined by atomic coordinates set forth in a table selected from Tables 1, 2, 3 and 4;

(ii) comparing the three-dimensional coordinates of the ligand when it is bound to KSP as set forth in Table 1, 2, 3 or 4 to the three-dimensional coordinates of a compound in a database of compound structures; and

(iii) selecting from said database at least one compound that is structurally similar to said ligand when it is bound to said KSP, wherein the selected compound is a potential inhibitor of said KSP.

Also provided is a method for identifying an anti-mitotic agent which upon binding to a target human KSP inhibits cell proliferation, the method comprising the steps of:

a) exposing a target KSP to a mixture of at least two potential ligands;

b) attempting to crystallize said target KSP in the presence of said mixture;

c) obtaining a crystal of said target KSP exposed to said mixture to determine whether ligand/KSP complex is formed; and

d) identifying a potential anti-mitotic agent as one that binds to said KSP at a ligand binding site having the relative structural coordinates as set forth in Table 5 ± the root mean square deviation of not more than about 2.0 Å.

Further provided is a method for identifying an anti-mitotic agent which upon binding to a target human KSP inhibits cell proliferation, the method comprising the steps of:

(a) obtaining a crystal of KSP, where said KSP has been crystallized while exposed to a mixture of at least two potential ligands;

(b) determining whether a ligand/KSP complex is formed in said crystal; and

(c) identifying a potential anti-mitotic agent as one that binds to said KSP at a ligand binding site having the relative structural coordinates as set forth in Table 5 ± the root mean square deviation of not more than about 2.0 Å.

In the methods described hereinabove, potential ligands of KSP include the test compounds and Mg++ and ADP.

Also provided is a method of modulating, e.g., inhibiting the activity of a KSP. The method can be *in vitro* or *in vivo*. The method comprises administering, *in vitro* or *in vivo*, a sufficient amount of a compound that binds to the binding site disclosed herein.

Also provided is a method of identifying a compound that selectively inhibits the activity of one type of KSP compared to other KSPs or kinesins, e.g., a KSP of one species over another or a KSP over another member of the BimC family, of which KSP is a member. Thus, the method enables the identification of KSP and KSP like proteins in the same family, e.g., BimC or the KSP in one species over another. The method is exemplified by modeling test compounds that fit spacially and preferentially into a KSP ligand binding site of interest using an atomic structural model of

a KSP ligand binding site, selecting a compound that interacts with one or more residues of the ligand binding site unique in the context of that site, and identifying in an assay for ligand binding activity a compound that selectively binds to the ligand binding site compared to other KSP. The unique features involved in receptor-selective ligand binding can be identified by comparing atomic models of different receptors or isoforms of the same type of receptor.

The present invention also provides for computer programs for the expression (such as visual display) of the KSP or analog three-dimensional structure, and further, a computer program which expresses the identity of each constituent of a KSP molecule and the precise location within the overall structure of that constituent, down to the atomic level.

There are many currently available computer programs for the expression of the three-dimensional structure of a molecule. Generally, these programs provide for inputting of the coordinates for the three-dimensional structure of a molecule (i.e., for example, a numerical assignment for each atom of a KSP molecule along an x, y, and z axis or the assignment for each atom of the binding site described in Tables 1-4), means to express (such as visually display) such coordinates, means to alter such coordinates and means to express an image of a molecule having such altered coordinates. One may program crystallographic information, i.e., the coordinates of the location of the atoms of a KSP binding site molecule in three dimension space, wherein such coordinates have been obtained from crystallographic analysis of said KSP molecule, into such programs to generate a computer program for the expression (such as visual display) of the KSP three-dimensional structure.

In furtherance of the above, the present invention provides a machine, such as a computer, programmed in memory with the coordinates of KSP or portions thereof, together with a program capable of converting the coordinates into a three-dimensional graphical representation of the structural coordinates on a display connected to the machine.

As well, there is provided a computer program for the expression of KSP's three-dimensional structure together with the structure of the novel KSP binding site. Preferred is the computer program QUANTA 2000, available from Molecular simulations or Insight II, version 4, available

from Biosym, San Diego, Calif., with the coordinates of the amino acids of Figure 10 as set forth in Tables 1-4 input. Preferred expression means are well known to a skilled artisan. Alternatively, the present KSP crystallographic coordinates and diffraction data are also deposited in the Protein Data Bank, Chemistry Department, Brookhaven National Laboratory, Upton, N.Y. 119723, USA. One may use these data in preparing a different computer program for expression of the three-dimensional structure of a KSP molecule or analog thereof.

Structural coordinates of a crystalline composition of this invention may be stored in a machine-readable form on a machine-readable storage medium, e.g. a computer hard drive, diskette, DAT tape, etc., for display as a three-dimensional shape or for other uses involving computer-assisted manipulation of, or computation based on, the structural coordinates or the three-dimensional structures they define. For example, data defining the three-dimensional structure of a KSP protein or portions or structurally similar homologues of such proteins, may be stored in a machine-readable storage medium, and may be displayed as a graphical three-dimensional representation of the protein structure, typically using a computer capable of reading the data from said storage medium and programmed with instructions for creating the representation from such data.

This invention thus encompasses a machine, such as a computer, having a memory which contains data representing the structural coordinates of a crystalline composition of this invention, e.g. the coordinates set forth in Tables 1-4, together with additional optional data and instructions for manipulating such data. Such data may be used for a variety of purposes, such as the elucidation of other related structures and drug discovery. For example, a machine having a memory containing such data aids in the rational design or selection of inhibitors of KSP binding or activity, including the evaluation of the ability of a particular chemical entity to favorably associate with KSP as disclosed herein, as well as in the modeling of compounds, proteins, complexes, etc. related by structural or sequence homology to KSP.

Thus, three-dimensional modeling of KSP provided by the present invention using the coordinates from the X-ray diffraction patterns can be entered into one or more computer programs for molecular modeling.

Such molecular modeling programs generate atomic coordinates that reflect the secondary, tertiary and/or quaternary structures of the protein which contribute to its overall three-dimensional structure and provide information related to binding and/or active sites of the protein.

The present invention further contemplates the use of the structural coordinates of the present invention with standard homology modeling techniques to determine the unknown three-dimensional structure of a target molecule or molecular complex. Homology modeling involves constructing a model of an unknown structure using structural coordinates of one or more related protein molecules/molecular complexes or parts thereof (i.e., ligand binding sites). In general, homology modeling entails fitting common or homologous portions of the protein whose three-dimensional structure is to be solved to the three-dimensional structure of homologous structural elements in the known molecule, specifically using the relevant (i.e., homologous) structural coordinates provided in Tables 1-4. Homology may be determined using amino acid sequence identity, homologous secondary structure elements, and/or homologous tertiary folds. Homology modeling can include rebuilding part or all of a three-dimensional structure with replacement of amino acids (or other components) by those of the related structure to be solved. Examples of programs for homology modeling include, but are not limited to: QUANTA (Molecular Simulations, Inc.), Molecular Operating Environment or MOE (Chemical Computing Group, Inc. 2002), MODELLER (copyright © 1989-2002 Andrej Sali; Departments of Biopharmaceutical Sciences and Pharmaceutical Chemistry, and California Institute for Quantitative Biomedical Research, Mission Bay Genentech Hall, University of California San Francisco) and others.

In accordance with the above, a three-dimensional structure for the unknown molecule/molecular complex may be generated using the three-dimensional structure of the KSP molecule of the present invention, Tables 1-4, refined using a number of techniques well known in the art, and then used in the same fashion as the structural coordinates of the present invention, for instance, in applications involving molecular replacement analysis, homology modeling, and rational drug design.

Among other aspects, the coordinates in Table 1-4 define the relative relationship between the protein, the nucleotide and the ligand. Such sets of

coordinates are dependent upon the particular coordinate system used. Those skilled in the art will recognize that rotation, translation or other mathematical manipulation of these coordinates may change the specific values of these coordinates, but the new set(s) will still define the relationship between the multiple components of the crystal structure disclosed herein."

The determination of the three-dimensional structure of the ligand binding site of KSP as disclosed herein is advantageous over conventional drug assay techniques, in which the only way to identify such an agent is to screen thousands of test compounds until an agent having the desired inhibitory effect on a target compound is identified. Generally, such conventional screening methods are expensive, time consuming, and do not elucidate the method of action of the identified agent on the target compound. In sharp contrast, advancing X-ray, spectroscopic and computer modeling technologies allow researchers to visualize the three-dimensional structure of a targeted compound (i.e., KSP ligand binding site), and using such a three-dimensional structure to identify putative binding sites and then identify or design agents to interact with these binding sites. These agents can thereafter be screened for an inhibitory effect upon the target molecule. Consequently, an embodiment of the invention details a method for identifying a potential inhibitor of KSP. The proposed method comprises using a three-dimensional structure of KSP and the novel binding site of the invention as defined by the relative structural coordinates of Tables 1-4 and the relative structural coordinates of the amino acid residues of Figure 10 as set forth in Table 1-4 to design or select a potential inhibitor of KSP activity, followed by synthesizing or obtaining the said potential inhibitor. The inhibitor may be selected by screening an appropriate database. Alternatively, it may be designed de novo by analyzing the steric configurations and charge potentials of a ligand bound KSP complex in conjunction with the appropriate software programs, or may be designed using characteristics of known inhibitors of KSP.

An entity/agent that interacts or associates with the ligand binding site of KSP may be identified by performing computer fitting analyses to identify an agent which interacts or associates with said site. Computer fitting analyses utilize various computer software programs that evaluate the "fit" between the binding site and the identified agent, by (a)

generating a three-dimensional model of the ligand binding site using homology modeling or the atomic structural coordinates of the binding site in Tables 1-4, and (b) determining the degree of association between the binding site and the identified agent. The degree of association may be determined computationally by any number of commercially available software programs, or may be determined experimentally using standard binding assays.

Preferably, the method of the present invention includes the use of a ligand binding site characterized by the three-dimensional structure comprising the relative structural coordinates of amino acid residues listed in Figure 10 as set forth in Tables 1-4 ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2.0 Å, preferably not more than about 1.0 Å, and most preferably not more than about 0.5 Å. It is understood that the method of the present invention includes additional embodiments comprising conservative substitutions of the noted amino acids which result in the same structural coordinates of the corresponding residues in Tables 1-4 within the stated root mean square deviation.

The effect of an agent identified by computer fitting analyses on human KSP activity may be further evaluated computationally, or experimentally by competitive binding experiments or by contacting the identified agent with KSP and measuring the effect of the agent on the target's biological activity. Standard enzymatic assays may be performed and the results analyzed to determine whether the agent is an inhibitor of KSP activity (i.e., induce cell cycle arrest or inhibit the association of KSP with a microtubule as well as any other known activities attending a kinesin). Further tests may be performed to evaluate the selectivity of the identified agent to KSP with regard to other KSP proteins (other species) or other members of the BimC protein family.

Preferably, the agent designed or selected to interact with KSP is capable of associating with KSP and of assuming a three-dimensional configuration and orientation that complements the relevant ligand binding site of KSP.

Consequently, using these criteria, the structural coordinates of the KSP molecule as disclosed herein, and/or structural coordinates

derived therefrom using molecular replacement or homology modeling, agents may be designed having increased potency and/or selectivity versus known inhibitors, e.g, by modifying the structure of known inhibitors or by designing new agents de novo via computational inspection of the three-dimensional configuration of KSP's novel ligand binding site described herein (relative structural coordinates of amino acid residues listed in Figure 10 as set forth in Tables 1-4 and the relative structural coordinates set forth in Table 5).

As such, an embodiment of the invention proposes using the structural coordinates of Tables 1-4 of the present invention, or structural coordinates derived therefrom using molecular replacement or homology modeling techniques as discussed above to screen a database for agents that may act as potential inhibitors of KSP activity. As an example, the obtained structural coordinates of the present invention may be read into a software package and the three-dimensional structure analyzed graphically. A number of computational software packages may be used for the analysis of structural coordinates, e.g., Sybyl (Tripos Associates) etc. Additional software programs may be optionally used to check the coordinates with regard to features such as bond and atom types. If necessary, the three-dimensional structure may be modified and then energy minimized using the appropriate software until all of the structural parameters are at their equilibrium/optimal values. The energy minimized structure can then be superimposed against the original structure to make sure there are no significant deviations between the original and the energy minimized coordinates.

Once the specific interaction between KSP and a known inhibitor is determined, e.g., such as the information provided in Tables 1-4, docking studies with different inhibitors will allow one skilled in the art to generate initial models of new inhibitors bound to KSP. The integrity of these new models may be evaluated a number of ways, including constrained conformational analysis using molecular dynamics methods; that is where both KSP and the bound inhibitor are allowed to sample different three-dimensional conformational states until the most favorable state is reached or found to exist between the protein and the bound agent etc. Once models are obtained of the original known agent bound to KSP

(Tables 1-4) and computer models of other molecules bound to KSP are as well obtained, strategies may be proposed determined for designing modifications into the inhibitors to improve their activity and/or enhance their selectivity.

For example, once a KSP binding agent has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its selectivity and binding properties for KSP. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. Such substituted chemical compounds may then be analyzed for efficiency of fit to KSP by the same computer methods described in detail above. Further molecular analysis and rational drug design techniques are disclosed in U.S. Pat. Nos. 5,834,228, and 5,939,528 the contents of which are incorporated by reference in their entirety.

Thus, an exemplary embodiment of the invention envisions a method of three-dimensional modeling of a KSP protein, comprising the steps of:

(a) providing three-dimensional atomic coordinates derived from X-ray diffraction measurements of a KSP protein in a computer readable format;

(b) inputting the data from step (a) into a computer with appropriate software programs; and

(c) generating a three-dimensional structural representation of the KSP protein suitable for visualization and further computational manipulation.

This invention further provides for the use of the structural coordinates of a crystalline composition of this invention, or portions thereof, to identify reactive amino acids within the three-dimensional structure, preferably within or adjacent to a ligand binding site; to generate and visualize a molecular surface, such as a water-accessible surface or a surface comprising the space-filling van der Waals surface of all atoms; to calculate and visualize the size and shape of surface features of the protein or complex, e.g., ligand binding pockets; to locate potential H-bond donors and acceptors within the three-dimensional structure, preferably within or

adjacent to a ligand binding site; to calculate regions of hydrophobicity and hydrophilicity within the three-dimensional structure, preferably within or adjacent to a ligand binding site; and to calculate and visualize regions on or adjacent to the protein surface of favorable interaction energies with respect to selected functional groups of interest (e.g. amino, hydroxyl, carboxyl, methylene, alkyl, alkenyl, aromatic carbon, aromatic rings, heteroaromatic rings, substituted and unsubstituted phosphates, substituted and unsubstituted phosphonates, substituted and unsubstituted fluoro and difluorophosphonates; etc.). One may use the foregoing approaches for characterizing the protein and its interactions with moieties of potential ligands to design or select compounds capable of specific covalent attachment to reactive amino acids (e.g., cysteine) and to design or select compounds of complementary characteristics (e.g., size, shape, charge, hydrophobicity/hydrophilicity, ability to participate in hydrogen bonding, etc.) to surface features of the protein, a set of which may be preselected. Using the structural coordinates, one may also predict or calculate the orientation, binding constant or relative affinity of a given ligand to the protein in the complexed state, and use that information to design or select compounds of improved affinity.

In such cases, the structural coordinates of the KSP protein, or portion or complex thereof, are entered in machine readable form into a machine programmed with instructions for carrying out the desired operation and containing any necessary additional data, e.g. data defining structural and/or functional characteristics of a potential ligand or moiety thereof, defining molecular characteristics of the various amino acids, etc.

The present invention is additionally directed to a method of determining the three-dimensional structure of a molecule or molecular complex whose structure is unknown, comprising the steps of first obtaining crystals of the molecule or molecular complex whose structure is unknown, and then generating X-ray diffraction data from the crystallized molecule or molecular complex and/or generating NMR data from the solution of the molecule or molecular complex. The generated diffraction or spectroscopy data from the molecule or molecular complex can then be compared with the solution coordinates or three-dimensional structure of KSP as disclosed herein, and the three-dimensional structure of the unknown molecule or

molecular complex conformed to the KSP structure using standard techniques such as molecular replacement analysis, 2D, 3D and 4D isotope filtering, editing and triple resonance NMR techniques, and computer homology modeling. Alternatively, a three-dimensional model of the unknown molecule may be generated by generating a sequence alignment between KSP and the unknown molecule, based on any or all of amino acid sequence identity, secondary structure elements or tertiary folds, and then generating by computer modeling a three-dimensional structure for the molecule using the three-dimensional structure of, and sequence alignment with, KSP.

Preferred embodiments of the aforementioned methods are those methods wherein the KSP protein comprises a binding site characterized by amino acid residues described in Figure 10.

This invention also provides peptidomimetic methods for designing a compound capable of binding to a KSP protein or KSP homolog. One such method involves graphically displaying a three-dimensional representation based on coordinates defining the three-dimensional structure of a KSP family protein or a portion thereof complexed with a ligand. Interactions between portions of a ligand and the protein may then be analyzed in order to identify candidate moieties for replacement. One or more portions of the ligand which interact with the protein may be replaced with substitute moieties selected from a knowledge base of one or more candidate substitute moieties, and/or moieties may be added to the ligand to permit additional interactions with the protein.

In another aspect of the instant invention, the structural coordinates of a crystalline composition of this invention, or portions thereof, may be used to identify one or more pharmacophores of a chemical compound that binds to the ligand binding site. Such a pharmacophore is described as a set of atoms, chemical groups, pseudo-atoms or vectors, and the relative positions in space of each of these pharmacophore features. Each feature, alone or in combination with its relative position, forms a pharmacophore parameter. Thus, the pharmacophore includes the pharmacophore features, and the relative position of each descriptor with regard to all other descriptors comprising the pharmacophore.

Pharmacophore models can be constructed either directly or indirectly. In the direct method, the pharmacophore feature spatial centers are inferred from

studying the X-ray structural coordinates or NMR structure of a receptor-ligand complex, followed by a shape-complementarity function analysis of the receptor binding site, usually performed using a computer and a computer-readable medium. In the indirect method, the structure of the receptor is unknown and the pharmacophore feature spatial centers are inferred by overlaying the three-dimensional conformations of active compounds and finding the common, overlapping functional groups.

The pharmacophore models of the present invention, obtained by combining both direct and indirect methods, are herein described, by way of example only and without any intention of being limiting, with reference to Figures 14A and B.

The first model pharmacophore (FIG. 14A) is represented by three pharmacophore features having the planar orientation shown: a sphere indicating the center of an aryl, heteroaryl or cycloalkyl ring (or, in general, of a hydrophobic group), and two small boxes (labeled HA and HD), representing the heterocenters of a hydrogen bond acceptor and a hydrogen bond donor, respectively. The second model pharmacophore (FIG. 14B) is represented by three pharmacophore features: two spheres indicating the centers of two aryl, heteroaryl or cycloalkyl rings (or hydrophobic groups in general), and a small box representing the heteroatomic center of a hydrogen bond acceptor (HA).

As used herein, "aryl" is intended to mean any stable monocyclic or bicyclic carbon ring of up to 7 atoms in each ring, wherein at least one ring is aromatic. Examples of such aryl elements include phenyl, naphthyl, tetrahydronaphthyl, indanyl and biphenyl. In cases where the aryl substituent is bicyclic and one ring is non-aromatic, it is understood that attachment is via the aromatic ring.

The term heteroaryl, as used herein, represents a stable monocyclic or bicyclic ring of up to 7 atoms in each ring, wherein at least one ring is aromatic and contains from 1 to 4 heteroatoms selected from the group consisting of O, N and S. Heteroaryl groups within the scope of this definition include but are not limited to: acridinyl, carbazolyl, cinnolinyl, quinoxalinyl, pyrrazolyl, indolyl, benzotriazolyl, furanyl, thienyl, benzothienyl, benzofuranyl, quinolinyl, isoquinolinyl, oxazolyl, isoxazolyl, indolyl, pyrazinyl, pyridazinyl, pyridinyl, pyrimidinyl, pyrrolyl, tetrahydroquinoline. In an embodiment of the instant invention, heteroaryl does not include quinazolinone.

As used herein, "cycloalkyl" is intended to include monocyclic saturated aliphatic hydrocarbon groups having the specified number of carbon atoms.

For example, "cycloalkyl" includes cyclopropyl, methyl-cyclopropyl, 2,2-dimethyl-cyclobutyl, 2-ethyl-cyclopentyl, cyclohexyl, and so on. In an embodiment of the invention the term "cycloalkyl" includes the groups described immediately above and further includes monocyclic unsaturated aliphatic hydrocarbon groups. For example, "cycloalkyl" as defined in this embodiment includes cyclopropyl, methyl-cyclopropyl, 2,2-dimethyl-cyclobutyl, 2-ethyl-cyclopentyl, cyclohexyl, cyclopentenyl, cyclobutenyl and so on.

The, cycloalkyl, aryl, heteroaryl and heteroaryl substituents may be substituted or unsubstituted, unless specifically defined otherwise. For example, an aryl may be substituted with one, two or three substituents selected from OH, alkyl, halogen, alkoxy or dialkylamino.

The active structural motifs designated herein as the model pharmacophores of the present invention can be used to screen libraries of molecules for the existence of a predefined structural motif, and in particular identifying molecules that meet the constraints imposed by the pharmacophore. The pharmacophore feature spatial centers are globally associated with a specific biological activity. The molecules being evaluated may be designed *de novo* using computer methods, or alternatively, be either a scaffold or a full chemical entity (e.g., chosen from a library of compounds). Using the model pharmacophores disclosed herein one of ordinary skill may predict the inhibitory potency of a compound based upon its fit with any of these two pharmacophore models shown in FIG. 14A and B.

In an embodiment, the compound identified by the use of a pharmacophore model described herein has a binding affinity for KSP of about 0.1 nM to about 100 nM. In a further embodiment, the binding affinity range is from about 1 nM to about 20 nM.

In an embodiment, the compound identified by its fit with the pharmacophore model of Figure 14A does not incorporate a 2-thioxo-1,2,3,4-tetrahydropyrimidine moiety, a dihydropyrimidine moiety or a 5,6,11,11a-tetrahydro-1H-imidazo[1',5':1,6]-pyrido[3.4-b]indole-1,3(2H)-dione moiety.

An additional pharmacophore model is illustrated by Figure 16. The pharmacophore model of Figure 16 is represented by four pharmacophore features: three spheres indicating the centers of aryl, heteroaryl or cycloalkyl rings (or hydrophobic groups in general), and a small box representing the heteroatomic center of a hydrogen bond acceptor (HA). In reference to Figure 16, the distances in Å between the pharmacophore features are listed in the following table:

	1	2	3	4
1	-			
2	5.1±0.6	-		
3	8.5±0.7	6.9±0.7	-	
4	3.7±0.5	5.8±0.6	5.7±0.7	-

In an embodiment, the compound identified by its fit with the pharmacophore model of Figure 16 does not incorporate a quinazolinone, phenothiazine, thienopyrimidinone, furanopyrimidinone, azolopyrimidinone, thiazolopyrimidine, cycloalkylpyrimidinone or triphenylmethane moiety. In a further embodiment, the compound identified by its fit with the pharmacophore model of Figure 16 does not incorporate a quinazolinone, phenothiazine or triphenylmethane moiety.

In an embodiment, the compound identified by its fit with the pharmacophore model of Figure 14B does not incorporate a quinazolinone, phenothiazine, thienopyrimidinone, furanopyrimidinone, azolopyrimidinone, thiazolopyrimidine, cycloalkylpyrimidinone or triphenylmethane moiety. In a further embodiment, the compound identified by its fit with the pharmacophore model of Fig. 14B does not incorporate a quinazolinone, phenothiazine or triphenylmethane moiety.

The degree of fit of a particular compound structure to the pharmacophore models is calculated by determining, using computer methods, if the compound possesses the chemical features of the pharmacophore model and if the features can adopt the necessary three-dimensional arrangement to fit the model. The modeling program will indicate those features in the pharmacophore model having a fit with the particular compound or chemical feature of the compound being tested. The term "fit" when referring to a compound and a pharmacophore or binding site includes both compounds that occupy only the spatial area of the pharmacophore or binding site and compounds of which the chemical features or a portion of the molecule occupy the spatial area of the pharmacophore or binding site.

Fitting of a compound to the ligand binding site volume can be done in a number of different ways using computational methods well known by those skilled in the art. Visual inspection and manual docking of compounds into the induced-fit active site volume can be done using molecular modeling software such as QUANTA (Molecular Simulations, Burlington, MA, 1992), SYBYL (Tripos Associates, Inc., St. Louis, MO, 1992), AMBER (Weiner et al., J. Am. Chem. Soc., 106: 765-784, 1984), CHARMM (Brooks et al., J. Comp. Chem., 4: 187-217, 1983) or other modeling

programs known to those of skill in the art. This modeling step may be followed by energy minimization using standard force fields, such as CHARMM and AMBER, or others. More specialized modeling programs include MCSS (Miranker & Karplus, Function and Genetics, 11: 29-34, 1991), GRID (Goodford et al., J. Med. Chem., 28: 849-857, 1985), AUTODOCK (Goodsell & Olsen, Proteins: Structure, Function and Genetics, 8: 195-202, 1990), and DOCK (Kuntz et al., J. Mol. Biol., 161: 269-288, 1982). In addition, inhibitor compounds may be constructed *de novo* in the empty active site or in the active site including some portions of a known inhibitor using computer programs such as LEGEND (Nishibata & Itai, Tetrahedron, 47: 8985, 1991), LeapFrog (Tripos Associates, St. Louis, MO), LUDI (Bohm, J. Comp. Aid. Molec. Design, 6: 61-78, 1992), AutoLudi (Accelrys Inc., San Diego, CA) or others.

Another aspect of the invention relates to a complementary protein having a structure substantially complementary to the three-dimensional structure according to Tables 1-4; or to a medicinally effective part thereof, particularly a ligand binding region. A complementary protein is one whose three-dimensional structure is substantially complementary to the Tables 1-4 structure or a part thereof, such that the complementary structure may bind thereto and may form a complex. The lifetime of the complex may be long in the case of an inhibiting complementary protein. Of course, binding will also require an appropriate choice of amino acid sequence. Such a complementary protein may act as an inhibitor of KSP. Such inhibitors may be used *in vivo* or *in vitro* to modify the activity of KSP.

In the pharmaceutical industry, new or known compounds are routinely screened for new uses employing a variety of known *in vitro* or *in vivo* screens. Often such screens involve complex natural substances and are correspondingly expensive to carry out, and the result may be difficult to interpret. The knowledge of the three-dimensional protein structure according to the invention allows a preliminary screening to be carried out on the basis of the three-dimensional structure of a region thereof, and the structural similarity of a molecule which is being screened. This is usually carried out in conjunction with a knowledge of the amino sequence of the region. Such screening can conveniently be carried out using computer modeling techniques, which match the three-dimensional structure of the protein or part thereof (or complementary protein or part thereof) with the

structure of the molecule being screened, thereby allowing one to predict potential inhibitor activity.

The binding of a ligand to the novel binding site of the instant invention and the formation of the novel binding pocket as a result can also be indirectly assessed by spectroscopically determining the shift in the fluorescence of the amino acid 127 tryptophan residue. Thus it has been discovered that the fluorescent emission of Trp127 is modulated when KSP is treated with one of the inhibitors described above in the presence of a nucleotide or nucleotides.

A further embodiment of the instant invention is an *in vitro* assay for the determination of binding of a test compound to the novel KSP binding site described herein. The assay comprises the steps of:

1. contacting KSP with the test compound and a nucleotide and measuring the fluorescence of the mixture at the peak emission wavelength for Trp127 in KSP;
2. contacting KSP with a nucleotide and measuring the fluorescence of the mixture at the peak emission wavelength for Trp127 in KSP; and
3. comparing the fluorescence of the mixture of KSP, the test compound and the nucleotide with the fluorescence of the mixture of KSP with the nucleotide alone.

In another embodiment of the *in vitro* fluorescence assay the nucleotide is selected from ADP and AMPPNP (a non-hydrolysable analog of ATP, adenosine 5'-(β,γ-imido)triphosphate tetralithium salt hydrate).

In an embodiment of the *in vitro* fluorescence assay the mixtures additionally contain a source of magnesium ion. Preferably the source of magnesium ion is $MgCl_2$.

In another embodiment of the *in vitro* fluorescence assay the measurement of the fluorescence of the KSP, test compound and nucleotide mixture is performed at several different concentrations of the test compound.

Because the KSP kinesin's three-dimensional structure is uniquely suited to the formation of the novel binding pocket of the instant invention, the methods of identification of compounds that bind to the novel binding pocket described herein, such as the fluorescence assay described

above, may be used to identify selective inhibitors of KSP which may not inhibit other mitotic kinesins. Such identification of a selective KSP inhibitor may offer particular advantages over an inhibitor which is competitive with the binding of the nucleotide substrate of KSP or which binds to the site of microtubule binding.

A still further aspect of the invention relates to antibodies (including monoclonal antibodies) directed to the KSP protein or complementary protein, for the detection thereof or for the modulation of its medicinal activity, it being understood that the antibody is specific for the KSP-ligand, e.g., inhibitor bound conformation.

Compounds of the structures selected or designed by any of the foregoing means may be tested for their ability to bind to a KSP protein, inhibit the binding of a KSP protein to a natural or non-natural ligand therefor, and/or inhibit a biological function mediated by a KSP protein or a BimC family member.

Finally, the present invention provides agents or inhibitors designed or selected using the methods disclosed herein. Such compounds may be utilized as described in the following sections.

Utilities

The compounds designed or selected using the methods of the invention find use in a variety of applications. As will be appreciated by those in the art, mitosis may be altered in a variety of ways; that is, one can affect mitosis either by increasing or decreasing the activity of a component in the mitotic pathway. Stated differently, mitosis may be affected (e.g., disrupted) by disturbing equilibrium, either by inhibiting or activating certain components. Similar approaches may be used to alter meiosis.

In a preferred embodiment, the compounds designed or selected using the methods of the invention are used to modulate mitotic spindle formation, thus causing prolonged cell cycle arrest in mitosis. By "modulate" herein is meant altering mitotic spindle formation, including increasing and decreasing spindle formation. By "mitotic spindle formation" herein is meant organization of microtubules into bipolar structures by mitotic kinesins. By "mitotic spindle dysfunction" herein is meant mitotic arrest and monopolar spindle formation.

The compounds designed or selected using the methods of the invention are useful to bind to and/or modulate the activity of a mitotic kinesin. In a

preferred embodiment, the mitotic kinesin is a member of the bimC subfamily of mitotic kinesins (as described in U.S. Patent No. 6,284,480, column 5). In a further preferred embodiment, the mitotic kinesin is human KSP, although the activity of mitotic kinesins from other organisms may also be modulated by the compounds of the present invention. In this context, modulate means either increasing or decreasing spindle pole separation, causing malformation, i.e., splaying, of mitotic spindle poles, or otherwise causing morphological perturbation of the mitotic spindle. Also included within the definition of KSP for these purposes are variants and/or fragments of KSP. See PCT Publ. WO 01/31335: "Methods of Screening for Modulators of Cell Proliferation and Methods of Diagnosing Cell Proliferation States", filed Oct. 27, 1999, hereby incorporated by reference in its entirety. In addition, other mitotic kinesins may be inhibited by the compounds of the present invention.

The compounds designed or selected using the methods of the invention are used to treat cellular proliferation diseases. Disease states which can be treated by the methods and compositions provided herein include, but are not limited to, cancer (further discussed below), autoimmune disease, arthritis, graft rejection, inflammatory bowel disease, proliferation induced after medical procedures, including, but not limited to, surgery, angioplasty, and the like. It is appreciated that in some cases the cells may not be in a hyper- or hypoproliferation state (abnormal state) and still require treatment. For example, during wound healing, the cells may be proliferating "normally", but proliferation enhancement may be desired. Similarly, as discussed above, in the agriculture arena, cells may be in a "normal" state, but proliferation modulation may be desired to enhance a crop by directly enhancing growth of a crop, or by inhibiting the growth of a plant or organism which adversely affects the crop. Thus, in one embodiment, the invention herein includes application to cells or individuals afflicted or impending affliction with any one of these disorders or states.

The compounds, compositions and methods provided herein are particularly deemed useful for the treatment of cancer including solid tumors such as skin, breast, brain, cervical carcinomas, testicular carcinomas, etc. More particularly, cancers that may be treated by the compounds, compositions and methods of the invention include, but are not limited to: Cardiac: sarcoma (angiosarcoma, fibrosarcoma, rhabdomyosarcoma, liposarcoma), myxoma, rhabdomyoma, fibroma, lipoma and teratoma; Lung: bronchogenic carcinoma (squamous cell, undifferentiated small cell, undifferentiated large cell, adenocarcinoma), alveolar (bronchiolar)

carcinoma, bronchial adenoma, sarcoma, lymphoma, chondromatous hamartoma, mesothelioma; Gastrointestinal: esophagus (squamous cell carcinoma, adenocarcinoma, leiomyosarcoma, lymphoma), stomach (carcinoma, lymphoma, leiomyosarcoma), pancreas (ductal adenocarcinoma, insulinoma, glucagonoma, gastrinoma, carcinoid tumors, vipoma), small bowel (adenocarcinoma, lymphoma, carcinoid tumors, Karposi's sarcoma, leiomyoma, hemangioma, lipoma, neurofibroma, fibroma), large bowel (adenocarcinoma, tubular adenoma, villous adenoma, hamartoma, leiomyoma); Genitourinary tract: kidney (adenocarcinoma, Wilm's tumor [nephroblastoma], lymphoma, leukemia), bladder and urethra (squamous cell carcinoma, transitional cell carcinoma, adenocarcinoma), prostate (adenocarcinoma, sarcoma), testis (seminoma, teratoma, embryonal carcinoma, teratocarcinoma, choriocarcinoma, sarcoma, interstitial cell carcinoma, fibroma, fibroadenoma, adenomatoid tumors, lipoma); Liver: hepatoma (hepatocellular carcinoma), cholangiocarcinoma, hepatoblastoma, angiosarcoma, hepatocellular adenoma, hemangioma; Bone: osteogenic sarcoma (osteosarcoma), fibrosarcoma, malignant fibrous histiocytoma, chondrosarcoma, Ewing's sarcoma, malignant lymphoma (reticulum cell sarcoma), multiple mycloma, malignant giant cell tumor chordoma, osteochronfroma (osteocartilaginous exostoses), benign chondroma, chondroblastoma, chondromyxofibroma, osteoid osteoma and giant cell tumors; Nervous system: skull (osteoma, hemangioma, granuloma, xanthoma, osteitis deformans), meninges (meningioma, meningiosarcoma, gliomatosis), brain (astrocytoma, medulloblastoma, glioma, ependymoma, germinoma [pinealoma], glioblastoma multiform, oligodendroglioma, schwannoma, retinoblastoma, congenital tumors), spinal cord neurofibroma, meningioma, glioma, sarcoma); Gynecological: uterus (endometrial carcinoma), cervix (cervical carcinoma, pre-tumor cervical dysplasia), ovaries (ovarian carcinoma [serous cystadenocarcinoma, mucinous cystadenocarcinoma, unclassified carcinoma], granulosa-thecal cell tumors, Sertoli-Leydig cell tumors, dysgerminoma, malignant teratoma), vulva (squamous cell carcinoma, intraepithelial carcinoma, adenocarcinoma, fibrosarcoma, melanoma), vagina (clear cell carcinoma, squamous cell carcinoma, botryoid sarcoma (embryonal rhabdomyosarcoma), fallopian tubes (carcinoma); Hematologic: blood (myeloid leukemia [acute and chronic], acute lymphoblastic leukemia, chronic lymphocytic leukemia, myeloproliferative diseases, multiple myeloma, myelodysplastic syndrome), Hodgkin's disease, non-Hodgkin's lymphoma [malignant lymphoma]; Skin: malignant melanoma, basal cell carcinoma, squamous cell carcinoma, Karposi's sarcoma, moles

dysplastic nevi, lipoma, angioma, dermatofibroma, keloids, psoriasis; and Adrenal glands: neuroblastoma. Thus, the term "cancerous cell" as provided herein, includes a cell afflicted by any one of the above-identified conditions.

The compounds designed or selected using the methods of the instant invention may also be useful as antifungal agents, by modulating the activity of the fungal members of the bimC kinesin subgroup, as is described in U.S. Patent No. 6,284,480.

The compounds designed or selected using the methods of this invention may be administered to mammals, preferably humans, either alone or, preferably, in combination with pharmaceutically acceptable carriers, excipients or diluents, in a pharmaceutical composition, according to standard pharmaceutical practice. The compounds can be administered orally or parenterally, including the intravenous, intramuscular, intraperitoneal, subcutaneous, rectal and topical routes of administration.

As used herein, the term "composition" is intended to encompass a product comprising the specified ingredients in the specific amounts, as well as any product which results, directly or indirectly, from combination of the specific ingredients in the specified amounts.

The pharmaceutical compositions containing the active ingredient may be in a form suitable for oral use, for example, as tablets, troches, lozenges, aqueous or oily suspensions, dispersible powders or granules, emulsions, hard or soft capsules, or syrups or elixirs. Compositions intended for oral use may be prepared according to any method known to the art for the manufacture of pharmaceutical compositions and such compositions may contain one or more agents selected from the group consisting of sweetening agents, flavoring agents, coloring agents and preserving agents in order to provide pharmaceutically elegant and palatable preparations. Tablets contain the active ingredient in admixture with non-toxic pharmaceutically acceptable excipients which are suitable for the manufacture of tablets. These excipients may be for example, inert diluents, such as calcium carbonate, sodium carbonate, lactose, calcium phosphate or sodium phosphate; granulating and disintegrating agents, for example, microcrystalline cellulose, sodium crosscarmellose, corn starch, or alginic acid; binding agents, for example starch, gelatin, polyvinyl-pyrrolidone or acacia, and lubricating agents, for example, magnesium stearate, stearic acid or talc. The tablets may be uncoated or they may be coated by known techniques to mask the unpleasant taste of the drug or delay disintegration and absorption in the gastrointestinal tract and

thereby provide a sustained action over a longer period. For example, a water soluble taste masking material such as hydroxypropyl-methylcellulose or hydroxypropylcellulose, or a time delay material such as ethyl cellulose, cellulose acetate buryrate may be employed.

Formulations for oral use may also be presented as hard gelatin capsules wherein the active ingredient is mixed with an inert solid diluent, for example, calcium carbonate, calcium phosphate or kaolin, or as soft gelatin capsules wherein the active ingredient is mixed with water soluble carrier such as polyethyleneglycol or an oil medium, for example peanut oil, liquid paraffin, or olive oil.

Aqueous suspensions contain the active material in admixture with excipients suitable for the manufacture of aqueous suspensions. Such excipients are suspending agents, for example sodium carboxymethylcellulose, methylcellulose, hydroxypropylmethyl-cellulose, sodium alginate, polyvinyl-pyrrolidone, gum tragacanth and gum acacia; dispersing or wetting agents may be a naturally-occurring phosphatide, for example lecithin, or condensation products of an alkylene oxide with fatty acids, for example polyoxyethylene stearate, or condensation products of ethylene oxide with long chain aliphatic alcohols, for example heptadecaethyleneoxycetanol, or condensation products of ethylene oxide with partial esters derived from fatty acids and a hexitol such as polyoxyethylene sorbitol monooleate, or condensation products of ethylene oxide with partial esters derived from fatty acids and hexitol anhydrides, for example polyethylene sorbitan monooleate. The aqueous suspensions may also contain one or more preservatives, for example ethyl, or n-propyl p-hydroxybenzoate, one or more coloring agents, one or more flavoring agents, and one or more sweetening agents, such as sucrose, saccharin or aspartame.

Oily suspensions may be formulated by suspending the active ingredient in a vegetable oil, for example arachis oil, olive oil, sesame oil or coconut oil, or in mineral oil such as liquid paraffin. The oily suspensions may contain a thickening agent, for example beeswax, hard paraffin or cetyl alcohol. Sweetening agents such as those set forth above, and flavoring agents may be added to provide a palatable oral preparation. These compositions may be preserved by the addition of an anti-oxidant such as butylated hydroxyanisol or alpha-tocopherol.

Dispersible powders and granules suitable for preparation of an aqueous suspension by the addition of water provide the active ingredient in

admixture with a dispersing or wetting agent, suspending agent and one or more preservatives. Suitable dispersing or wetting agents and suspending agents are exemplified by those already mentioned above. Additional excipients, for example sweetening, flavoring and coloring agents, may also be present. These compositions may be preserved by the addition of an anti-oxidant such as ascorbic acid.

The pharmaceutical compositions of the invention may also be in the form of an oil-in-water emulsions. The oily phase may be a vegetable oil, for example olive oil or arachis oil, or a mineral oil, for example liquid paraffin or mixtures of these. Suitable emulsifying agents may be naturally occurring phosphatides, for example soy bean lecithin, and esters or partial esters derived from fatty acids and hexitol anhydrides, for example sorbitan monooleate, and condensation products of the said partial esters with ethylene oxide, for example polyoxyethylene sorbitan monooleate. The emulsions may also contain sweetening, flavoring agents, preservatives and antioxidants.

Syrups and elixirs may be formulated with sweetening agents, for example glycerol, propylene glycol, sorbitol or sucrose. Such formulations may also contain a demulcent, a preservative, flavoring and coloring agents and antioxidant.

The pharmaceutical compositions may be in the form of a sterile injectable aqueous solutions. Among the acceptable vehicles and solvents that may be employed are water, Ringer's solution and isotonic sodium chloride solution.

The sterile injectable preparation may also be a sterile injectable oil-in-water microemulsion where the active ingredient is dissolved in the oily phase. For example, the active ingredient may be first dissolved in a mixture of soybean oil and lecithin. The oil solution then introduced into a water and glycerol mixture and processed to form a microemulation.

The injectable solutions or microemulsions may be introduced into a patient's blood stream by local bolus injection. Alternatively, it may be advantageous to administer the solution or microemulsion in such a way as to maintain a constant circulating concentration of the instant compound. In order to maintain such a constant concentration, a continuous intravenous delivery device may be utilized. An example of such a device is the Deltec CADD-PLUS™ model 5400 intravenous pump.

The pharmaceutical compositions may be in the form of a sterile injectable aqueous or oleagenous suspension for intramuscular and subcutaneous administration. This suspension may be formulated according to the known art using

those suitable dispersing or wetting agents and suspending agents which have been mentioned above. The sterile injectable preparation may also be a sterile injectable solution or suspension in a non-toxic parenterally acceptable diluent or solvent, for example as a solution in 1,3-butane diol. In addition, sterile, fixed oils are conventionally employed as a solvent or suspending medium. For this purpose any bland fixed oil may be employed including synthetic mono- or diglycerides. In addition, fatty acids such as oleic acid find use in the preparation of injectables.

Compounds designed or selected using the methods disclosed herein may also be administered in the form of suppositories for rectal administration of the drug. These compositions can be prepared by mixing the drug with a suitable non-irritating excipient which is solid at ordinary temperatures but liquid at the rectal temperature and will therefore melt in the rectum to release the drug. Such materials include cocoa butter, glycerinated gelatin, hydrogenated vegetable oils, mixtures of polyethylene glycols of various molecular weights and fatty acid esters of polyethylene glycol.

For topical use, creams, ointments, jellies, solutions or suspensions, etc., containing the compound are employed. (For purposes of this application, topical application shall include mouth washes and gargles.)

The compounds designed or selected using the methods of the present invention can be administered in intranasal form via topical use of suitable intranasal vehicles and delivery devices, or via transdermal routes, using those forms of transdermal skin patches well known to those of ordinary skill in the art. To be administered in the form of a transdermal delivery system, the dosage administration will, of course, be continuous rather than intermittent throughout the dosage regimen. Compounds of the present invention may also be delivered as a suppository employing bases such as cocoa butter, glycerinated gelatin, hydrogenated vegetable oils, mixtures of polyethylene glycols of various molecular weights and fatty acid esters of polyethylene glycol.

When a compound according to this invention is administered into a human subject, the daily dosage will normally be determined by the prescribing physician with the dosage generally varying according to the age, weight, sex and response of the individual patient, as well as the severity of the patient's symptoms.

In one exemplary application, a suitable amount of compound is administered to a mammal undergoing treatment for cancer. Administration occurs in an amount between about 0.1 mg/kg of body weight to about 60 mg/kg of body

weight per day, preferably of between 0.5 mg/kg of body weight to about 40 mg/kg of body weight per day.

The compounds designed or selected using the methods disclosed herein (hereafter referred to as the "instant compounds") are also useful in combination with known therapeutic agents and anti-cancer agents. For example, instant compounds are useful in combination with known anti-cancer agents. Combinations of the presently disclosed compounds with other anti-cancer or chemotherapeutic agents are within the scope of the invention. Examples of such agents can be found in *Cancer Principles and Practice of Oncology* by V.T. Devita and S. Hellman (editors), 6th edition (February 15, 2001), Lippincott Williams & Wilkins Publishers. A person of ordinary skill in the art would be able to discern which combinations of agents would be useful based on the particular characteristics of the drugs and the cancer involved. Such anti-cancer agents include, but are not limited to, the following: estrogen receptor modulators, androgen receptor modulators, retinoid receptor modulators, cytotoxic/cytostatic agents, antiproliferative agents, prenyl-protein transferase inhibitors, HMG-CoA reductase inhibitors and other angiogenesis inhibitors, inhibitors of cell proliferation and survival signaling, and agents that interfere with cell cycle checkpoints. The instant compounds are particularly useful when co-administered with radiation therapy.

In an embodiment, the instant compounds are also useful in combination with known anti-cancer agents including the following: estrogen receptor modulators, androgen receptor modulators, retinoid receptor modulators, cytotoxic agents, antiproliferative agents, prenyl-protein transferase inhibitors, HMG-CoA reductase inhibitors, HIV protease inhibitors, reverse transcriptase inhibitors, and other angiogenesis inhibitors.

"Estrogen receptor modulators" refers to compounds that interfere with or inhibit the binding of estrogen to the receptor, regardless of mechanism. Examples of estrogen receptor modulators include, but are not limited to, tamoxifen, raloxifene, idoxifene, LY353381, LY117081, toremifene, fulvestrant, 4-[7-(2,2-dimethyl-1-oxopropoxy-4-methyl-2-[4-[2-(1-piperidinyl)ethoxy]phenyl]-2H-1-benzopyran-3-yl]-phenyl-2,2-dimethylpropanoate, 4,4'-dihydroxybenzophenone-2,4-dinitrophenyl-hydrazone, and SH646.

"Androgen receptor modulators" refers to compounds which interfere or inhibit the binding of androgens to the receptor, regardless of mechanism.

Examples of androgen receptor modulators include finasteride and other 5α-reductase inhibitors, nilutamide, flutamide, bicalutamide, liarozole, and abiraterone acetate.

"Retinoid receptor modulators" refers to compounds which interfere or inhibit the binding of retinoids to the receptor, regardless of mechanism. Examples of such retinoid receptor modulators include bexarotene, tretinoin, 13-cis-retinoic acid, 9-cis-retinoic acid, α-difluoromethylornithine, ILX23-7553, trans-N-(4'-hydroxyphenyl) retinamide, and N-4-carboxyphenyl retinamide.

"Cytotoxic/cytostatic agents" refer to compounds which cause cell death or inhibit cell proliferation primarily by interfering directly with the cell's functioning or inhibit or interfere with cell myosis, including alkylating agents, tumor necrosis factors, intercalators, hypoxia activatable compounds, microtubule inhibitors/microtubule-stabilizing agents, inhibitors of mitotic kinesins, inhibitors of kinases involved in mitotic progression, antimetabolites; biological response modifiers; hormonal/anti-hormonal therapeutic agents, haematopoietic growth factors, monoclonal antibody targeted therapeutic agents, topoisomerase inhibitors, proteosome inhibitors and ubiquitin ligase inhibitors.

Examples of cytotoxic agents include, but are not limited to, sertenef, cachectin, ifosfamide, tasonermin, lonidamine, carboplatin, altretamine, prednimustine, dibromodulcitol, ranimustine, fotemustine, nedaplatin, oxaliplatin, temozolomide, heptaplatin, estramustine, improsulfan tosilate, trofosfamide, nimustine, dibrospidium chloride, pumitepa, lobaplatin, satraplatin, profiromycin, cisplatin, irofulven, dexifosfamide, cis-aminedichloro(2-methyl-pyridine)platinum, benzylguanine, glufosfamide, GPX100, (trans, trans, trans)-bis-mu-(hexane-1,6-diamine)-mu-[diamine-platinum(II)]bis[diamine(chloro)platinum (II)]tetrachloride, diarizidinylspermine, arsenic trioxide, 1-(11-dodecylamino-10-hydroxyundecyl)-3,7-dimethylxanthine, zorubicin, idarubicin, daunorubicin, bisantrene, mitoxantrone, pirarubicin, pinafide, valrubicin, amrubicin, antineoplaston, 3'-deamino-3'-morpholino-13-deoxo-10-hydroxycarminomycin, annamycin, galarubicin, elinafide, MEN10755, and 4-demethoxy-3-deamino-3-aziridinyl-4-methylsulphonyl-daunorubicin (see WO 00/50032).

An example of a hypoxia activatable compound is tirapazamine.

Examples of proteosome inhibitors include but are not limited to lactacystin and MLN-341 (Velcade).

Examples of microtubule inhibitors/microtubule-stabilising agents include paclitaxel, vindesine sulfate, 3',4'-didehydro-4'-deoxy-8'-

norvincaleukoblastine, docetaxol, rhizoxin, dolastatin, mivobulin isethionate, auristatin, cemadotin, RPR109881, BMS184476, vinflunine, cryptophycin, 2,3,4,5,6-pentafluoro-N-(3-fluoro-4-methoxyphenyl) benzene sulfonamide, anhydrovinblastine, N,N-dimethyl-L-valyl-L-valyl-N-methyl-L-valyl-L-prolyl-L-proline-t-butylamide, TDX258, the epothilones (see for example U.S. Pat. Nos. 6,284,781 and 6,288,237) and BMS188797. In an embodiment the epothilones are not included in the microtubule inhibitors/microtubule-stabilising agents.

Some examples of topoisomerase inhibitors are topotecan, hycaptamine, irinotecan, rubitecan, 6-ethoxypropionyl-3',4'-O-exo-benzylidene-chartreusin, 9-methoxy-N,N-dimethyl-5-nitropyrazolo[3,4,5-kl]acridine-2-(6H) propanamine, 1-amino-9-ethyl-5-fluoro-2,3-dihydro-9-hydroxy-4-methyl-1H,12H-benzo[de]pyrano[3',4':b,7]-indolizino[1,2b]quinoline-10,13(9H,15H)dione, lurtotecan, 7-[2-(N-isopropylamino)ethyl]-(20S)camptothecin, BNP1350, BNPI1100, BN80915, BN80942, etoposide phosphate, teniposide, sobuzoxane, 2'-dimethylamino-2'-deoxy-etoposide, GL331, N-[2-(dimethylamino)ethyl]-9-hydroxy-5,6-dimethyl-6H-pyrido[4,3-b]carbazole-1-carboxamide, asulacrine, (5a, 5aB, 8aa,9b)-9-[2-[N-[2-(dimethylamino)ethyl]-N-methylamino]ethyl]-5-[4-hydro0xy-3,5-dimethoxyphenyl]-5,5a,6,8,8a,9-hexohydrofuro(3',4':6,7)naphtho(2,3-d)-1,3-dioxol-6-one, 2,3-(methylenedioxy)-5-methyl-7-hydroxy-8-methoxybenzo[c]-phenanthridinium, 6,9-bis[(2-aminoethyl)amino]benzo[g]isoguinoline-5,10-dione, 5-(3-aminopropylamino)-7,10-dihydroxy-2-(2-hydroxyethylaminomethyl)-6H-pyrazolo[4,5,1-de]acridin-6-one, N-[1-[2(diethylamino)ethylamino]-7-methoxy-9-oxo-9H-thioxanthen-4-ylmethyl]formamide, N-(2-(dimethylamino)ethyl)acridine-4-carboxamide, 6-[[2-(dimethylamino)ethyl]amino]-3-hydroxy-7H-indeno[2,1-c] quinolin-7-one, and dimesna.

Examples of inhibitors of mitotic kinesins, and in particular the human mitotic kinesin KSP, are described in PCT Publications WO 01/30768 and WO 01/98278, and pending U.S. Ser. Nos. 60/338,779 (filed December 6, 2001), 60/338,344 (filed December 6, 2001), 60/338,383 (filed December 6, 2001), 60/338,380 (filed December 6, 2001), 60/338,379 (filed December 6, 2001) and 60/344,453 (filed November 7, 2001). In an embodiment inhibitors of mitotic kinesins include, but are not limited to inhibitors of KSP, inhibitors of MKLP1, inhibitors of CENP-E, inhibitors of MCAK and inhibitors of Rab6-KIFL.

"Inhibitors of kinases involved in mitotic progression" include, but are not limited to, inhibitors of aurora kinase, inhibitors of Polo-like kinases (PLK) (in particular inhibitors of PLK-1), inhibitors of bub-1 and inhibitors of bub-R1.

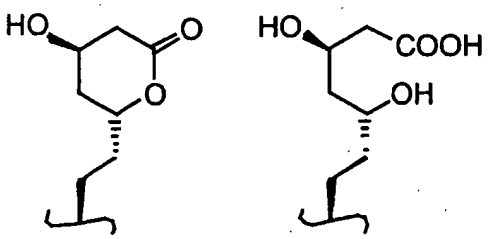
"Antiproliferative agents" includes antisense RNA and DNA oligonucleotides such as G3139, ODN698, RVASKRAS, GEM231, and INX3001, and antimetabolites such as enocitabine, carmofur, tegafur, pentostatin, doxifluridine, trimetrexate, fludarabine, capecitabine, galocitabine, cytarabine ocfosfate, fosteabine sodium hydrate, raltitrexed, paltitrexid, emitefur, tiazofurin, decitabine, nolatrexed, pemetrexed, nelzarabine, 2'-deoxy-2'-methylidenecytidine, 2'-fluoromethylene-2'-deoxycytidine, N-[5-(2,3-dihydro-benzofuryl)sulfonyl]-N'-(3,4-dichlorophenyl)urea, N6-[4-deoxy-4-[N2-[2(E),4(E)-tetradecadienoyl]glycylamino]-L-glycero-B-L-manno-heptopyranosyl]adenine, aplidine, ecteinascidin, troxacitabine, 4-[2-amino-4-oxo-4,6,7,8-tetrahydro-3H-pyrimidino[5,4-b][1,4]thiazin-6-yl-(S)-ethyl]-2,5-thienoyl-L-glutamic acid, aminopterin, 5-flurouracil, alanosine, 11-acetyl-8-(carbamoyloxymethyl)-4-formyl-6-methoxy-14-oxa-1,11-diazatetracyclo(7.4.1.0.0)-tetradeca-2,4,6-trien-9-yl acetic acid ester, swainsonine, lometrexol, dexrazoxane, methioninase, 2'-cyano-2'-deoxy-N4-palmitoyl-1-B-D-arabino furanosyl cytosine, 3-aminopyridine-2-carboxaldehyde thiosemicarbazone and trastuzumab.

Examples of monoclonal antibody targeted therapeutic agents include those therapeutic agents which have cytotoxic agents or radioisotopes attached to a cancer cell specific or target cell specific monoclonal antibody. Examples include Bexxar.

"HMG-CoA reductase inhibitors" refers to inhibitors of 3-hydroxy-3-methylglutaryl-CoA reductase. Compounds which have inhibitory activity for HMG-CoA reductase can be readily identified by using assays well-known in the art. For example, see the assays described or cited in U.S. Patent 4,231,938 at col. 6, and WO 84/02131 at pp. 30-33. The terms "HMG-CoA reductase inhibitor" and "inhibitor of HMG-CoA reductase" have the same meaning when used herein.

Examples of HMG-CoA reductase inhibitors that may be used include but are not limited to lovastatin (MEVACOR®; see U.S. Patent Nos. 4,231,938, 4,294,926 and 4,319,039), simvastatin (ZOCOR®; see U.S. Patent Nos. 4,444,784, 4,820,850 and 4,916,239), pravastatin (PRAVACHOL®; see U.S. Patent Nos. 4,346,227, 4,537,859, 4,410,629, 5,030,447 and 5,180,589), fluvastatin (LESCOL®; see U.S. Patent Nos. 5,354,772, 4,911,165, 4,929,437, 5,189,164, 5,118,853, 5,290,946 and 5,356,896), atorvastatin (LIPITOR®; see U.S. Patent Nos. 5,273,995,

4,681,893, 5,489,691 and 5,342,952) and cerivastatin (also known as rivastatin and BAYCHOL®; see US Patent No. 5,177,080). The structural formulas of these and additional HMG-CoA reductase inhibitors that may be used in the instant methods are described at page 87 of M. Yalpani, "Cholesterol Lowering Drugs", *Chemistry & Industry*, pp. 85-89 (5 February 1996) and US Patent Nos. 4,782,084 and 4,885,314. The term HMG-CoA reductase inhibitor as used herein includes all pharmaceutically acceptable lactone and open-acid forms (i.e., where the lactone ring is opened to form the free acid) as well as salt and ester forms of compounds which have HMG-CoA reductase inhibitory activity, and therefor the use of such salts, esters, open-acid and lactone forms is included within the scope of this invention. An illustration of the lactone portion and its corresponding open-acid form is shown below as structures I and II.



Lactone I

Open-Acid II

In HMG-CoA reductase inhibitors where an open-acid form can exist, salt and ester forms may be formed from the open-acid, and all such forms are included within the meaning of the term "HMG-CoA reductase inhibitor" as used herein. In an embodiment, the HMG-CoA reductase inhibitor is selected from lovastatin and simvastatin, and in a further embodiment, simvastatin. Herein, the term "pharmaceutically acceptable salts" with respect to the HMG-CoA reductase inhibitor shall mean non-toxic salts of the compounds employed in this invention which are generally prepared by reacting the free acid with a suitable organic or inorganic base, particularly those formed from cations such as sodium, potassium, aluminum, calcium, lithium, magnesium, zinc and tetramethylammonium, as well as those salts formed from amines such as ammonia, ethylenediamine, N-methylglucamine, lysine, arginine, ornithine, choline, N,N'-dibenzylethylenediamine, chloroprocaine, diethanolamine, procaine, N-benzylphenethylamine, 1-p-

chlorobenzyl-2-pyrrolidine-1'-yl-methylbenz-imidazole, diethylamine, piperazine, and tris(hydroxymethyl) aminomethane. Further examples of salt forms of HMG-CoA reductase inhibitors may include, but are not limited to, acetate, benzenesulfonate, benzoate, bicarbonate, bisulfate, bitartrate, borate, bromide, calcium edetate, camsylate, carbonate, chloride, clavulanate, citrate, dihydrochloride, edetate, edisylate, estolate, esylate, fumarate, gluceptate, gluconate, glutamate, glycollylarsanilate, hexylresorcinate, hydrabamine, hydrobromide, hydrochloride, hydroxynapthoate, iodide, isothionate, lactate, lactobionate, laurate, malate, maleate, mandelate, mesylate, methylsulfate, mucate, napsylate, nitrate, oleate, oxalate, pamaote, palmitate, panthothenate, phosphate/diphosphate, polygalacturonate, salicylate, stearate, subacetate, succinate, tannate, tartrate, teoclate, tosylate, triethiodide, and valerate.

Ester derivatives of the described HMG-CoA reductase inhibitor compounds may act as prodrugs which, when absorbed into the bloodstream of a warm-blooded animal, may cleave in such a manner as to release the drug form and permit the drug to afford improved therapeutic efficacy.

"Prenyl-protein transferase inhibitor" refers to a compound which inhibits any one or any combination of the prenyl-protein transferase enzymes, including farnesyl-protein transferase (FPTase), geranylgeranyl-protein transferase type I (GGPTase-I), and geranylgeranyl-protein transferase type-II (GGPTase-II, also called Rab GGPTase). Examples of prenyl-protein transferase inhibiting compounds include (±)-6-[amino(4-chlorophenyl)(1-methyl-1H-imidazol-5-yl)methyl]-4-(3-chlorophenyl)-1-methyl-2(1*H*)-quinolinone, (-)-6-[amino(4-chlorophenyl)(1-methyl-1H-imidazol-5-yl)methyl]-4-(3-chlorophenyl)-1-methyl-2(1*H*)-quinolinone, (+)-6-[amino(4-chlorophenyl)(1-methyl-1H-imidazol-5-yl) methyl]-4-(3-chlorophenyl)-1-methyl-2(1*H*)-quinolinone, 5(S)-n-butyl-1-(2,3-dimethylphenyl)-4-[1-(4-cyanobenzyl)-5-imidazolylmethyl]-2-piperazinone, (S)-1-(3-chlorophenyl) -4-[1-(4-cyanobenzyl)-5-imidazolylmethyl]-5-[2-(ethanesulfonyl) methyl)-2-piperazinone, 5(S)-n-Butyl-1-(2-methylphenyl)-4-[1-(4-cyanobenzyl)-5-imidazolylmethyl]-2-piperazinone, 1-(3-chlorophenyl) -4-[1-(4-cyanobenzyl)-2-methyl-5-imidazolylmethyl]-2-piperazinone, 1-(2,2-diphenylethyl)-3-[N-(1-(4-cyanobenzyl)-1H-imidazol-5-ylethyl)carbamoyl]piperidine, 4-{5-[4-hydroxymethyl-4-(4-chloropyridin-2-ylmethyl)-piperidine-1-ylmethyl]-2-methylimidazol-1-ylmethyl} benzonitrile, 4-{5-[4-hydroxymethyl-4-(3-chlorobenzyl)-piperidine-1-ylmethyl]-2-methylimidazol-1-ylmethyl}benzonitrile, 4-{3-[4-(2-oxo-2H-pyridin-1-yl)benzyl]-3H-

imidazol-4-ylmethyl}benzonitrile, 4-{3-[4-(5-chloro-2-oxo-2H-[1,2']bipyridin-5'-ylmethyl]-3H-imidazol-4-ylmethyl}benzonitrile, 4-{3-[4-(2-oxo-2H-[1,2'] bipyridin-5'-ylmethyl]-3H-imidazol-4-ylmethyl}benzonitrile, 4-[3-(2-oxo-1-phenyl-1,2-dihydropyridin-4-ylmethyl)-3H-imidazol-4-ylmethyl}benzonitrile, 18,19-dihydro-19-oxo-5*H*,17*H*-6,10:12,16-dimetheno-1H-imidazo[4,3-*c*][1,11,4]dioxaazacyclononadecine-9-carbonitrile, (±)-19,20-dihydro-19-oxo-5*H*-18,21-ethano-12,14-etheno-6,10-metheno-22*H*-benzo[*d*]imidazo[4,3-*k*][1,6,9,12]oxatriaza-cyclooctadecine-9-carbonitrile, 19,20-dihydro-19-oxo-5*H*,17*H*-18,21-ethano-6,10:12,16-dimetheno-22*H*-imidazo[3,4-*h*][1,8,11,14]oxatriazacycloeicosine-9-carbonitrile, and (±)-19,20-dihydro-3-methyl-19-oxo-5*H*-18,21-ethano-12,14-etheno-6,10-metheno-22*H*-benzo [*d*]imidazo[4,3-*k*][1,6,9,12]oxa-triazacyclooctadecine-9-carbonitrile.

Other examples of prenyl-protein transferase inhibitors can be found in the following publications and patents: WO 96/30343, WO 97/18813, WO 97/21701, WO 97/23478, WO 97/38665, WO 98/28980, WO 98/29119, WO 95/32987, U.S. Patent No. 5,420,245, U.S. Patent No. 5,523,430, U.S. Patent No. 5,532,359, U.S. Patent No. 5,510,510, U.S. Patent No. 5,589,485, U.S. Patent No. 5,602,098, European Patent Publ. 0 618 221, European Patent Publ. 0 675 112, European Patent Publ. 0 604 181, European Patent Publ. 0 696 593, WO 94/19357, WO 95/08542, WO 95/11917, WO 95/12612, WO 95/12572, WO 95/10514, U.S. Patent No. 5,661,152, WO 95/10515, WO 95/10516, WO 95/24612, WO 95/34535, WO 95/25086, WO 96/05529, WO 96/06138, WO 96/06193, WO 96/16443, WO 96/21701, WO 96/21456, WO 96/22278, WO 96/24611, WO 96/24612, WO 96/05168, WO 96/05169, WO 96/00736, U.S. Patent No. 5,571,792, WO 96/17861, WO 96/33159, WO 96/34850, WO 96/34851, WO 96/30017, WO 96/30018, WO 96/30362, WO 96/30363, WO 96/31111, WO 96/31477, WO 96/31478, WO 96/31501, WO 97/00252, WO 97/03047, WO 97/03050, WO 97/04785, WO 97/02920, WO 97/17070, WO 97/23478, WO 97/26246, WO 97/30053, WO 97/44350, WO 98/02436, and U.S. Patent No. 5,532,359.

For an example of the role of a prenyl-protein transferase inhibitor on angiogenesis see European J. of Cancer, Vol. 35, No. 9, pp.1394-1401 (1999).

"Angiogenesis inhibitors" refers to compounds that inhibit the formation of new blood vessels, regardless of mechanism. Examples of angiogenesis inhibitors include, but are not limited to, tyrosine kinase inhibitors, such as inhibitors of the tyrosine kinase receptors Flt-1 (VEGFR1) and Flk-1/KDR (VEGFR2), inhibitors of epidermal-derived, fibroblast-derived, or platelet derived growth factors,

MMP (matrix metalloprotease) inhibitors, integrin blockers, interferon-α, interleukin-12, pentosan polysulfate, cyclooxygenase inhibitors, including nonsteroidal anti-inflammatories (NSAIDs) like aspirin and ibuprofen as well as selective cyclooxygenase-2 inhibitors like celecoxib and rofecoxib (PNAS, Vol. 89, p. 7384 (1992); JNCI, Vol. 69, p. 475 (1982); Arch. Opthalmol., Vol. 108, p.573 (1990); Anat. Rec., Vol. 238, p. 68 (1994); FEBS Letters, Vol. 372, p. 83 (1995); Clin, Orthop. Vol. 313, p. 76 (1995); J. Mol. Endocrinol., Vol. 16, p.107 (1996); Jpn. J. Pharmacol., Vol. 75, p. 105 (1997); Cancer Res., Vol. 57, p. 1625 (1997); Cell, Vol. 93, p. 705 (1998); Intl. J. Mol. Med., Vol. 2, p. 715 (1998); J. Biol. Chem., Vol. 274, p. 9116 (1999)), steroidal anti-inflammatories (such as corticosteroids, mineralocorticoids, dexamethasone, prednisone, prednisolone, methylpred, betamethasone), carboxyamidotriazole, combretastatin A-4, squalamine, 6-O-chloroacetyl-carbonyl)-fumagillol, thalidomide, angiostatin, troponin-1, angiotensin II antagonists (see Fernandez et al., J. Lab. Clin. Med. 105:141-145 (1985)), and antibodies to VEGF (see, Nature Biotechnology, Vol. 17, pp.963-968 (October 1999); Kim et al., Nature, *362*, 841-844 (1993); WO 00/44777; and WO 00/61186).

Other therapeutic agents that modulate or inhibit angiogenesis and may also be used in combination with the compounds of the instant invention include agents that modulate or inhibit the coagulation and fibrinolysis systems (see review in *Clin. Chem. La. Med.* 38:679-692 (2000)). Examples of such agents that modulate or inhibit the coagulation and fibrinolysis pathways include, but are not limited to, heparin (see *Thromb. Haemost.* 80:10-23 (1998)), low molecular weight heparins, GPIIb/IIIa antagonists (such as tirofiban), warfarin, thrombin inhibitors and carboxypeptidase U inhibitors (also known as inhibitors of active thrombin activatable fibrinolysis inhibitor [TAFIa]) (see *Thrombosis Res.* 101:329-354 (2001)). TAFIa inhibitors have been described in U.S. Serial Nos. 60/310,927 (filed August 8, 2001) and 60/349,925 (filed January 18, 2002).

"Agents that interfere with cell cycle checkpoints" refer to compounds that inhibit protein kinases that transduce cell cycle checkpoint signals, thereby sensitizing the cancer cell to DNA damaging agents. Such agents include inhibitors of ATR, ATM, the Chk1 and Chk2 kinases and cdk and cdc kinase inhibitors and are specifically exemplified by 7-hydroxystaurosporin, flavopiridol, CYC202 (Cyclacel) and BMS-387032.

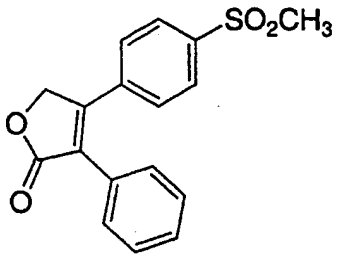
"Inhibitors of cell proliferation and survival signalling pathway" refer to compounds that inhibit signal transduction cascades downstream of cell surface receptors. Such agents include inhibitors of serine/threonine kinases (including but not limited to inhibitors of Akt such as described in WO 02/083064, WO 02/083139, WO 02/083140 and WO 02/083138), inhibitors of Raf kinase (for example BAY-43-9006), inhibitors of MEK (for example CI-1040 and PD-098059), inhibitors of mTOR (for example Wyeth CCI-779), and inhibitors of PI3K (for example LY294002).

The combinations with NSAID's are directed to the use of NSAID's which are potent COX-2 inhibiting agents. For purposes of this specification an NSAID is potent if it possess an IC_{50} for the inhibition of COX-2 of 1μM or less as measured by cell or microsomal assays.

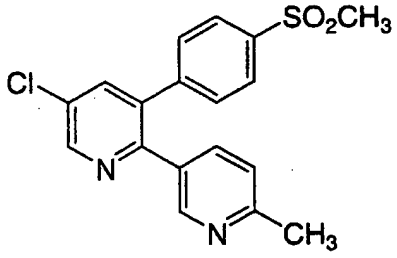
The invention also encompasses combinations with NSAID's which are selective COX-2 inhibitors. For purposes of this specification NSAID's which are selective inhibitors of COX-2 are defined as those which possess a specificity for inhibiting COX-2 over COX-1 of at least 100 fold as measured by the ratio of IC_{50} for COX-2 over IC_{50} for COX-1 evaluated by cell or microsomal assays. Such compounds include, but are not limited to those disclosed in U.S. Patent 5,474,995, issued December 12, 1995, U.S. Patent 5,861,419, issued January 19, 1999, U.S. Patent 6,001,843, issued December 14, 1999, U.S. Patent 6,020,343, issued February 1, 2000, U.S. Patent 5,409,944, issued April 25, 1995, U.S. Patent 5,436,265, issued July 25, 1995, U.S. Patent 5,536,752, issued July 16, 1996, U.S. Patent 5,550,142, issued August 27, 1996, U.S. Patent 5,604,260, issued February 18, 1997, U.S. 5,698,584, issued December 16, 1997, U.S. Patent 5,710,140, issued January 20,1998, WO 94/15932, published July 21, 1994, U.S. Patent 5,344,991, issued June 6, 1994, U.S. Patent 5,134,142, issued July 28, 1992, U.S. Patent 5,380,738, issued January 10, 1995, U.S. Patent 5,393,790, issued February 20, 1995, U.S. Patent 5,466,823, issued November 14, 1995, U.S. Patent 5,633,272, issued May 27, 1997, and U.S. Patent 5,932,598, issued August 3, 1999, all of which are hereby incorporated by reference.

Inhibitors of COX-2 that are particularly useful in the instant method of treatment are:

3-phenyl-4-(4-(methylsulfonyl)phenyl)-2-(*5H*)-furanone; and



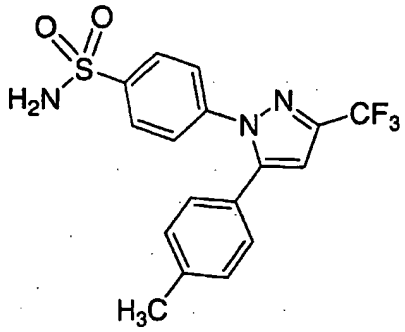
5-chloro-3-(4-methylsulfonyl)phenyl-2-(2-methyl-5-pyridinyl)pyridine;

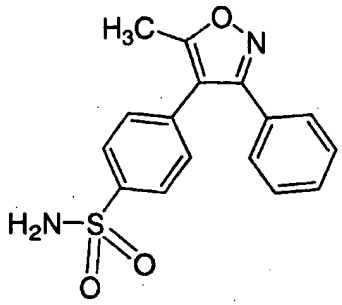


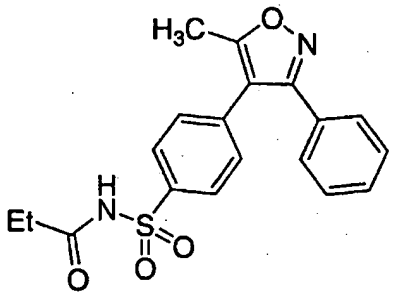
or a pharmaceutically acceptable salt thereof.

General and specific synthetic procedures for the preparation of the COX-2 inhibitor compounds described above are found in U.S. Patent No. 5,474,995, issued December 12, 1995, U.S. Patent No. 5,861,419, issued January 19, 1999, and U.S. Patent No. 6,001,843, issued December 14, 1999, all of which are herein incorporated by reference.

Compounds that have been described as specific inhibitors of COX-2 and are therefore useful in the present invention include, but are not limited to, the following:







or a pharmaceutically acceptable salt thereof.

Compounds which are described as specific inhibitors of COX-2 and are therefore useful in the present invention, and methods of synthesis thereof, can be found in the following patents, pending applications and publications, which are herein incorporated by reference: WO 94/15932, published July 21, 1994, U.S. Patent No. 5,344,991, issued June 6, 1994, U.S. Patent No. 5,134,142, issued July 28, 1992, U.S. Patent No. 5,380,738, issued January 10, 1995, U.S. Patent No. 5,393,790, issued February 20, 1995, U.S. Patent No. 5,466,823, issued November 14, 1995, U.S. Patent No. 5,633,272, issued May 27, 1997, and U.S. Patent No. 5,932,598, issued August 3, 1999.

Compounds which are specific inhibitors of COX-2 and are therefore useful in the present invention, and methods of synthesis thereof, can be found in the following patents, pending applications and publications, which are herein incorporated by reference: U.S. Patent No. 5,474,995, issued December 12, 1995, U.S. Patent No. 5,861,419, issued January 19, 1999, U.S. Patent No. 6,001,843, issued December 14, 1999, U.S. Patent No. 6,020,343, issued February 1, 2000, U.S. Patent No. 5,409,944, issued April 25, 1995, U.S. Patent No. 5,436,265, issued July 25, 1995, U.S. Patent No. 5,536,752, issued July 16, 1996, U.S. Patent No. 5,550,142, issued August 27, 1996, U.S. Patent No. 5,604,260, issued February 18, 1997, U.S. Patent No. 5,698,584, issued December 16, 1997, and U.S. Patent No. 5,710,140, issued January 20,1998.

Other examples of angiogenesis inhibitors include, but are not limited to, endostatin, ukrain, ranpirnase, IM862, 5-methoxy-4-[2-methyl-3-(3-methyl-2-butenyl)oxiranyl]-1-oxaspiro[2,5]oct-6-yl(chloroacetyl)carbamate, acetyldinanaline, 5-amino-1-[[3,5-dichloro-4-(4-chlorobenzoyl)phenyl]methyl]-1H-1,2,3-triazole-4-carboxamide,CM101, squalamine, combretastatin, RPI4610, NX31838, sulfated mannopentaose phosphate, 7,7-(carbonyl-bis[imino-N-methyl-4,2-pyrrolocarbonylimino[N-methyl-4,2-pyrrole]-carbonylimino]-bis-(1,3-naphthalene disulfonate), and 3-[(2,4-dimethylpyrrol-5-yl)methylene]-2-indolinone (SU5416).

As used above, "integrin blockers" refers to compounds which selectively antagonize, inhibit or counteract binding of a physiological ligand to the $\alpha_v\beta_3$ integrin, to compounds which selectively antagonize, inhibit or counteract binding of a physiological ligand to the $\alpha v\beta 5$ integrin, to compounds which antagonize, inhibit or counteract binding of a physiological ligand to both the $\alpha_v\beta_3$ integrin and the $\alpha_v\beta_5$ integrin, and to compounds which antagonize, inhibit or counteract the activity of the particular integrin(s) expressed on capillary endothelial cells. The term also refers to antagonists of the $\alpha_v\beta_6$, $\alpha_v\beta_8$, $\alpha_1\beta_1$, $\alpha_2\beta_1$, $\alpha_5\beta_1$, $\alpha_6\beta_1$ and $\alpha_6\beta_4$ integrins. The term also refers to antagonists of any combination of $\alpha_v\beta_3$, $\alpha_v\beta_5$, $\alpha_v\beta_6$, $\alpha_v\beta_8$, $\alpha_1\beta_1$, $\alpha_2\beta_1$, $\alpha_5\beta_1$, $\alpha_6\beta_1$ and $\alpha_6\beta_4$ integrins.

Some specific examples of tyrosine kinase inhibitors include N-(trifluoromethylphenyl)-5-methylisoxazol-4-carboxamide, 3-[(2,4-dimethylpyrrol-5-yl)methylidenyl)indolin-2-one, 17-(allylamino)-17-demethoxygeldanamycin, 4-(3-chloro-4-fluorophenylamino)-7-methoxy-6-[3-(4-morpholinyl)propoxyl]quinazoline, N-(3-ethynylphenyl)-6,7-bis(2-methoxyethoxy)-4-quinazolinamine, BIBX1382, 2,3,9,10,11,12-hexahydro-10-(hydroxymethyl)-10-hydroxy-9-methyl-9,12-epoxy-1H-

diindolo[1,2,3-fg:3',2',1'-kl]pyrrolo[3,4-i][1,6]benzodiazocin-1-one, SH268, genistein, STI571, CEP2563, 4-(3-chlorophenylamino)-5,6-dimethyl-7H-pyrrolo[2,3-d]pyrimidinemethane sulfonate, 4-(3-bromo-4-hydroxyphenyl)amino-6,7-dimethoxyquinazoline, 4-(4'-hydroxyphenyl)amino-6,7-dimethoxyquinazoline, SU6668, STI571A, N-4-chlorophenyl-4-(4-pyridylmethyl)-1-phthalazinamine, and EMD121974.

Combinations with compounds other than anti-cancer compounds are also encompassed in the instant methods. For example, combinations of the instantly claimed compounds with PPAR-γ (i.e., PPAR-gamma) agonists and PPAR-δ (i.e., PPAR-delta) agonists are useful in the treatment of certain malingnancies. PPAR-γ and PPAR-δ are the nuclear peroxisome proliferator-activated receptors γ and δ. The expression of PPAR-γ on endothelial cells and its involvement in angiogenesis has been reported in the literature (see *J. Cardiovasc. Pharmacol.* 1998; 31:909-913; *J. Biol. Chem.* 1999;274:9116-9121; *Invest. Ophthalmol Vis. Sci.* 2000; 41:2309-2317). More recently, PPAR-γ agonists have been shown to inhibit the angiogenic response to VEGF in vitro; both troglitazone and rosiglitazone maleate inhibit the development of retinal neovascularization in mice. (*Arch. Ophthamol.* 2001; 119:709-717). Examples of PPAR-γ agonists and PPAR-γ/α agonists include, but are not limited to, thiazolidinediones (such as DRF2725, CS-011, troglitazone, rosiglitazone, and pioglitazone), fenofibrate, gemfibrozil, clofibrate, GW2570, SB219994, AR-H039242, JTT-501, MCC-555, GW2331, GW409544, NN2344, KRP297, NP0110, DRF4158, NN622, GI262570, PNU182716, DRF552926, 2-[(5,7-dipropyl-3-trifluoromethyl-1,2-benzisoxazol-6-yl)oxy]-2-methylpropionic acid (disclosed in USSN 09/782,856), and 2(R)-7-(3-(2-chloro-4-(4-fluorophenoxy) phenoxy)propoxy)-2-ethylchromane-2-carboxylic acid (disclosed in USSN 60/235,708 and 60/244,697).

Another embodiment of the instant invention is the use of the presently disclosed compounds in combination with gene therapy for the treatment of cancer. For an overview of genetic strategies to treating cancer see Hall et al (*Am J Hum Genet* 61:785-789, 1997) and Kufe et al (*Cancer Medicine*, 5th Ed, pp 876-889, BC Decker, Hamilton 2000). Gene therapy can be used to deliver any tumor suppressing gene. Examples of such genes include, but are not limited to, p53, which can be delivered via recombinant virus-mediated gene transfer (see U.S. Patent No. 6,069,134, for example), a uPA/uPAR antagonist ("Adenovirus-Mediated Delivery of a uPA/uPAR Antagonist Suppresses Angiogenesis-Dependent Tumor Growth and

Dissemination in Mice," *Gene Therapy*, August 1998;5(8):1105-13), and interferon gamma (*J Immunol* 2000;164:217-222).

The compounds designed or selected using the methods of the instant invention may also be administered in combination with an inhibitor of inherent multidrug resistance (MDR), in particular MDR associated with high levels of expression of transporter proteins. Such MDR inhibitors include inhibitors of p-glycoprotein (P-gp), such as LY335979, XR9576, OC144-093, R101922, VX853 and PSC833 (valspodar).

A compound designed or selected using the methods of the present invention may be employed in conjunction with anti-emetic agents to treat nausea or emesis, including acute, delayed, late-phase, and anticipatory emesis, which may result from the use of a compound of the present invention, alone or with radiation therapy. For the prevention or treatment of emesis, a compound of the present invention may be used in conjunction with other anti-emetic agents, especially neurokinin-1 receptor antagonists, 5HT3 receptor antagonists, such as ondansetron, granisetron, tropisetron, and zatisetron, GABAB receptor agonists, such as baclofen, a corticosteroid such as Decadron (dexamethasone), Kenalog, Aristocort, Nasalide, Preferid, Benecorten or others such as disclosed in U.S.Patent Nos. 2,789,118, 2,990,401, 3,048,581, 3,126,375, 3,929,768, 3,996,359, 3,928,326 and 3,749,712, an antidopaminergic, such as the phenothiazines (for example prochlorperazine, fluphenazine, thioridazine and mesoridazine), metoclopramide or dronabinol. For the treatment or prevention of emesis that may result upon administration of the instant compounds, conjunctive therapy with an anti-emesis agent selected from a neurokinin-1 receptor antagonist, a 5HT3 receptor antagonist and a corticosteroid is preferred.

Neurokinin-1 receptor antagonists of use in conjunction with the compounds of the present invention are fully described, for example, in U.S. Patent Nos. 5,162,339, 5,232,929, 5,242,930, 5,373,003, 5,387,595, 5,459,270, 5,494,926, 5,496,833, 5,637,699, 5,719,147; European Patent Publication Nos. EP 0 360 390, 0 394 989, 0 428 434, 0 429 366, 0 430 771, 0 436 334, 0 443 132, 0 482 539, 0 498 069, 0 499 313, 0 512 901, 0 512 902, 0 514 273, 0 514 274, 0 514 275, 0 514 276, 0 515 681, 0 517 589, 0 520 555, 0 522 808, 0 528 495, 0 532 456, 0 533 280, 0 536 817, 0 545 478, 0 558 156, 0 577 394, 0 585 913,0 590 152, 0 599 538, 0 610 793, 0 634 402, 0 686 629, 0 693 489, 0 694 535, 0 699 655,

0 699 674, 0 707 006, 0 708 101, 0 709 375, 0 709 376, 0 714 891, 0 723 959, 0 733 632 and 0 776 893; PCT International Patent Publication Nos. WO 90/05525, 90/05729, 91/09844, 91/18899, 92/01688, 92/06079, 92/12151, 92/15585, 92/17449, 92/20661, 92/20676, 92/21677, 92/22569, 93/00330, 93/00331, 93/01159, 93/01165, 93/01169, 93/01170, 93/06099, 93/09116, 93/10073, 93/14084, 93/14113, 93/18023, 93/19064, 93/21155, 93/21181, 93/23380, 93/24465, 94/00440, 94/01402, 94/02461, 94/02595, 94/03429, 94/03445, 94/04494, 94/04496, 94/05625, 94/07843, 94/08997, 94/10165, 94/10167, 94/10168, 94/10170, 94/11368, 94/13639, 94/13663, 94/14767, 94/15903, 94/19320, 94/19323, 94/20500, 94/26735, 94/26740, 94/29309, 95/02595, 95/04040, 95/04042, 95/06645, 95/07886, 95/07908, 95/08549, 95/11880, 95/14017, 95/15311, 95/16679, 95/17382, 95/18124, 95/18129, 95/19344, 95/20575, 95/21819, 95/22525, 95/23798, 95/26338, 95/28418, 95/30674, 95/30687, 95/33744, 96/05181, 96/05193, 96/05203, 96/06094, 96/07649, 96/10562, 96/16939, 96/18643, 96/20197, 96/21661, 96/29304, 96/29317, 96/29326, 96/29328, 96/31214, 96/32385, 96/37489, 97/01553, 97/01554, 97/03066, 97/08144, 97/14671, 97/17362, 97/18206, 97/19084, 97/19942 and 97/21702; and in British Patent Publication Nos. 2 266 529, 2 268 931, 2 269 170, 2 269 590, 2 271 774, 2 292 144, 2 293 168, 2 293 169, and 2 302 689. The preparation of such compounds is fully described in the aforementioned patents and publications, which are incorporated herein by reference.

In an embodiment, the neurokinin-1 receptor antagonist for use in conjunction with the compounds of the present invention is selected from: 2-(R)-(1-(R)-(3,5-bis(trifluoromethyl)phenyl)ethoxy)-3-(S)-(4-fluorophenyl)-4-(3-(5-oxo-1H,4H-1,2,4-triazolo)methyl)morpholine, or a pharmaceutically acceptable salt thereof, which is described in U.S. Patent No. 5,719,147.

A compound designed or selected using the methods of the instant invention may also be administered with an agent useful in the treatment of anemia. Such an anemia treatment agent is, for example, a continuous eythropoiesis receptor activator (such as epoetin alfa).

A compound designed or selected using the methods of the instant invention may also be administered with an agent useful in the treatment of neutropenia. Such a neutropenia treatment agent is, for example, a hematopoietic growth factor which regulates the production and function of neutrophils such as a human granulocyte colony stimulating factor, (G-CSF). Examples of a G-CSF include filgrastim.

A compound designed or selected using the methods of the instant invention may also be administered with an immunologic-enhancing drug, such as levamisole, isoprinosine and Zadaxin.

Thus, the scope of the instant invention encompasses the use of the compounds designed or selected using the methods disclosed herein in combination with a second compound selected from:

1) an estrogen receptor modulator,
2) an androgen receptor modulator,
3) retinoid receptor modulator,
4) a cytotoxic/cytostatic agent,
5) an antiproliferative agent,
6) a prenyl-protein transferase inhibitor,
7) an HMG-CoA reductase inhibitor,
8) an HIV protease inhibitor,
9) a reverse transcriptase inhibitor,
10) an angiogenesis inhibitor,
11) a PPAR-γ agonists,
12) a PPAR-δ agonists,
13) an inhibitor of inherent multidrug resistance,
14) an anti-emetic agent,
15) an agent useful in the treatment of anemia,
16) an agent useful in the treatment of neutropenia,
17) an immunologic-enhancing drug,
18) an inhibitor of cell proliferation and survival signaling, and
19) an agent that interfers with a cell cycle checkpoint.

The term "administration" and variants thereof (e.g., "administering" a compound) in reference to a compound of the invention means introducing the compound or a prodrug of the compound into the system of the animal in need of treatment. When a compound of the invention or prodrug thereof is provided in combination with one or more other active agents (e.g., a cytotoxic agent, etc.), "administration" and its variants are each understood to include concurrent and sequential introduction of the compound or prodrug thereof and other agents.

As used herein, the term "composition" is intended to encompass a product comprising the specified ingredients in the specified amounts, as well as any

product which results, directly or indirectly, from combination of the specified ingredients in the specified amounts.

The term "therapeutically effective amount" as used herein means that amount of active compound or pharmaceutical agent that elicits the biological or medicinal response in a tissue, system, animal or human that is being sought by a researcher, veterinarian, medical doctor or other clinician.

The term "treating cancer" or "treatment of cancer" refers to administration to a mammal afflicted with a cancerous condition and refers to an effect that alleviates the cancerous condition by killing the cancerous cells, but also to an effect that results in the inhibition of growth and/or metastasis of the cancer.

In an embodiment, the angiogenesis inhibitor to be used as the second compound is selected from a tyrosine kinase inhibitor, an inhibitor of epidermal-derived growth factor, an inhibitor of fibroblast-derived growth factor, an inhibitor of platelet derived growth factor, an MMP (matrix metalloprotease) inhibitor, an integrin blocker, interferon-α, interleukin-12, pentosan polysulfate, a cyclooxygenase inhibitor, carboxyamidotriazole, combretastatin A-4, squalamine, 6-O-chloroacetyl-carbonyl)-fumagillol, thalidomide, angiostatin, troponin-1, or an antibody to VEGF. In an embodiment, the estrogen receptor modulator is tamoxifen or raloxifene.

Also included in the scope of the claims is a method of treating cancer that comprises administering a therapeutically effective amount of a compound designed or selected using the methods disclosed herein in combination with radiation therapy and/or in combination with a compound selected from:

1) an estrogen receptor modulator,
2) an androgen receptor modulator,
3) a retinoid receptor modulator,
4) a cytotoxic/cytostatic agent,
5) an antiproliferative agent,
6) a prenyl-protein transferase inhibitor,
7) an HMG-CoA reductase inhibitor,
8) an HIV protease inhibitor,
9) a reverse transcriptase inhibitor,
10) an angiogenesis inhibitor,
11) PPAR-γ agonists,
12) PPAR-δ agonists,
13) an inhibitor of inherent multidrug resistance,

14) an anti-emetic agent,
15) an agent useful in the treatment of anemia,
16) an agent useful in the treatment of neutropenia,
17) an immunologic-enhancing drug,
18) an inhibitor of cell proliferation and survival signaling, and
19) an agent that interfers with a cell cycle checkpoint.

And yet another embodiment of the invention is a method of treating cancer that comprises administering a therapeutically effective amount of a compound designed or selected using the methods disclosed herein in combination with paclitaxel or trastuzumab.

The invention further encompasses a method of treating or preventing cancer that comprises administering a therapeutically effective amount of a compound designed or selected using the methods disclosed herein in combination with a COX-2 inhibitor.

The instant invention also includes a pharmaceutical composition useful for treating or preventing cancer that comprises a therapeutically effective amount of a compound designed or selected using the methods disclosed herein and a compound selected from:

1) an estrogen receptor modulator,
2) an androgen receptor modulator,
3) a retinoid receptor modulator,
4) a cytotoxic/cytostatic agent,
5) an antiproliferative agent,
6) a prenyl-protein transferase inhibitor,
7) an HMG-CoA reductase inhibitor,
8) an HIV protease inhibitor,
9) a reverse transcriptase inhibitor,
10) an angiogenesis inhibitor, and
11) a PPAR-γ agonist,
12) a PPAR-δ agonists;
13) an inhibitor of cell proliferation and survival signaling, and
14) an agent that interfers with a cell cycle checkpoint.

In each of the aforementioned uses of atomic coordinates of KSP, the coordinates according to Tables 1-4 are preferred.

Additional objects of the present invention will be apparent from the description which follows.

As used herein, the following terms and phrases shall have the meanings set forth below:

Unless otherwise noted, "KSP" includes both native and wild type Kinesin Spindle Protein as well as "KSP analogues", defined herein as proteins or peptides comprising a ligand binding site substantially as set forth in SEQ ID NO:1. Such KSP analogues include, but are not limited to, a ligand binding site characterized by a three-dimensional structure comprising the relative structural coordinates of amino acid residues set forth in Figure 10 as set forth in Tables 1-4, ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than 3.005 Å, more preferably not more than about 2.0Å, and most preferably not more than about 0.5 Å.

Unless otherwise indicated, "protein" or "molecule" shall include a protein, protein domain, polypeptide or peptide.

"Structural coordinates" are the Cartesian coordinates corresponding to an atom's spatial relationship to other atoms in a molecule or molecular complex. Structural coordinates may be obtained using X-ray crystallography techniques or NMR techniques, or may be derived using molecular replacement analysis or homology modeling. Various software programs allow for the graphical representation of a set of structural coordinates to obtain a three-dimensional representation of a molecule or molecular complex. The structural coordinates of the present invention may be modified from the original sets provided in Tables 1-4 by mathematical manipulation, such as by inversion or integer additions or subtractions. As such, it is recognized that the structural coordinates of the present invention are relative, and are in no way specifically limited by the actual x, y, z coordinates of Tables 1-4.

An "agent", "ligand" or "binding partner" shall include a protein, polypeptide, peptide, nucleic acid, including DNA or RNA, molecule, compound or drug.

"Root mean square deviation" is the square root of the arithmetic mean of the squares of the deviations from the mean, and is a way of expressing deviation or variation from the structural coordinates

described herein. The present invention includes all embodiments comprising conservative substitutions of the noted amino acid residues resulting in same structural coordinates within the stated root mean square deviation.

MATERIALS AND METHODS

Materials and methods provided are intended to assist in a further understanding of the invention and are not to limit the reasonable scope thereof.

Motor Domain of Human KSP, Amino Acids 1-368

MASQPNSSAK KKEEKGKNIQ VVVRCRPFNL AERKASAHSI VECDPVRKEV SVRTGGLADK SSRKTYTFDM VFGASTKQID VYRSVVCPIL DEVIMGYNCT IFAYGQTGTG KTFTMEGERS PNEEYTWEED PLAGIIPRTL HQIFEKLTDN GTEFSVKVSL LEIYNEELFD LLNPSSDVSE RLQMFDDPRN KRGVIIKGLE EITVHNKDEV YQILEKGAAK RTTAATLMNA YSSRSHSVFS VTIHMKETTI DGEELVKIGK LNLVDLAGSE NIGRSGAVDK RAREAGNINQ SLLTLGRVIT ALVERTPHVP YRESKLTRIL QDSLGGRTRT SIIATISPAS LNLEETLSTL EYAHRAKNIL NKPEVNQK

Binding Pocket of Human KSP

Lining the newly formed pocket and surrounding the ligand are amino acid residues:

115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P) (from helix-α2 and its insertion loop; residue 116 is at the end of the first portion of helix-α2 and residue 134 is at the beginning of the second portion of helix-α2 thus the insertion loop starts at residue 116 and ends at residue 134);

160(L) (from beta strain-β4);

211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) (from helix-α3); and

239(F) (from beta strain-β6).

KSP Expression

E. coli cells harboring the KSP (368 residues) vector were grown at 37°C in LB medium containing 100 µg/ml ampicillin. KSP expression was induced at 25°C with 0.5mM isopropyl-D (–)-thiogalactopyranoside, and the cells were grown for four additional hours at 25°C prior to harvest.

Cells from 10 litre were suspended in 75 ml lysis buffer (50mM PIPES, 2mM $MgCl_2$, 1mM ATP, 1mM TCEP, 1mM EGTA, protease inhibitor tablets (one tablet per 50ml buffer)) and homogenized. Cells were disrupted by passing the homogenized suspension thrice through a Microfluidizer (Model 110-S). The cell lysate was centrifuged at 15,000 rpm for 30 minutes and the supernatant mixed with DE-52 resin (100 ml) pre-equilibrated in SP sepharose Buffer A (50mM PIPES, 2mM $MgCl_2$, 1mM ATP, 1mM TCEP, 1mM EGTA). Supernatant was removed after spinning at 1000 rpm for 10 minutes. Resin was washed twice with one resin volume (100ml) of 50mM PIPES, 2mM $MgCl_2$, 1mM ATP, 1mM TCEP, 1mM EGTA. The supernatants were pooled and loaded onto SP sepharose column (50ml, 2.6cm diameter column, Amersham Biosciences). Kinesin with ~95% purity was eluted at 0.15 to 0.2 M KCl using 0-30% KCl gradient. The fractions containing KSP (by SDS-PAGE analysis) were pooled and diluted with SP sepharose buffer A to a final KCl concentration of 50mM. The pool was mixed with 10ml of High performance Q-sepharose (Amersham Biosciencs) equilibrated in SP sepharose BufferA. The supernatent was collected by spinning at 1000rpm for 10 minutes. The resin was washed four times with two resin volume. The washes and supernatant were pooled and concentrated on Centriprep-10 to 15 to 17mg/ml and stored in small alicots at -70° C. The protein was characterized by N-terminal sequence analysis by Edman degradation on an Applied Biosystem model 470A gas phase sequencer. Protein concentration was determined with quantitative amino acid analysis by using a post column ninhydrin derivatization method on a Beckman 6300 analyzer. Molecular weight was determined on Deca-LCQ (Finnegan) mass spectrometer. Molar mass and size distribution was determined by multi-angle light scattering detector (Wyatt technology, DAWN EOS) connected to size exclusion column on Millenium HPLC.

Crystallization

The concentrated kinesin (ADP, Mg^{++}) protein at about 15mg/ml in 50mM PIPES buffer at pH 6.8 in the presence of 2mM $MgCl_2$, 1mM TECP, 1mM ATP, 84mM KCl, and 1mM EGTA was incubated with 1mM inhibitor Compound 5-2b ((+)-monastrol). Small single crystal seeds were obtained by hanging drop method with well solution containing 20% PEG3350, 0.15M K_2HPO_4 and 0.1M HEPES buffer at pH7.0 in about four days. Crystals suitable for X-ray data collection were obtained by macro-seeding in hanging drops with well solution containing 14% PEG3350, 0.2M K_2HPO_4 and 0.1M HEPES at pH 6.8 in about two weeks. Hanging drops were formed by equal volume of protein and well solutions.

X-ray Data Collection and Procession

The X-ray diffraction data at 2.5 Å resolution were collected at 100K at synchrotron beamline 17-ID of the Advanced Photon Source at Argonne National Laboratory. Prior to data collection the crystal was soaked in the cryo-protectant solution for 20 minutes that contains 20% PEG3350, 0.15M K_2HPO_4, 20% PEG200, and 0.1M HEPES buffer at pH6.8. The crystal was then frozen in liquid nitrogen. The X-ray wavelength was set to 1Å. The data were collected at 0.2° oscillation per frame with 1000 frames total and 1 second exposure per frame at 250 mm detector to crystal distance. The data were processed and scaled by use of HKL2000 package. The crystal is in orthorhombic space group of $P2_12_12_1$ with cell dimensions of a= 69.5 Å b=79.5 Å and c=159.0 Å. The completeness of the data set was 99%. The Rsym was 0.084.

Structure Determination and Refinement

The structure was determined by the use of the molecular replacement method in cooperation with extensive model rebuilding and dynamic refinement. The kinesin protein coordinates in the binary complex crystal structure of kinesin bound with ADP (Mg^{++}) was used as the search model. The molecular replacement solution was obtained with use of program AmoRe at 4.0Å to 15Å resolution range, which gave R-factor of 0.48 and correlation coefficient of 0.60. The initial protein model was

rebuilt and refined literally at 2.5Å resolution, those included dynamic refinement, energy minimization and temperature factor refinement. The Compound 5-2b density became apparent at the fourth rebuilding and refinement cycle. Finally, 441 water molecules were added in the model and the R-factor was 0.21 with R-free of 0.26 with good geometry ($RMSD_{bonds}$ = 0.007 Å, $RMSD_{angles}$ = 1.32 °). The current protein model binds with one ADP, one Mg^{++} ion and one Compound 5-2b. It starts at residue Asn18 to Lys362 with a gap from residue Asn271 to Asn287 (missing loop11 from Ile272 to Gly286) due to lack of electron density. There are two complexes in an asymmetric unit.

Tertiary Structure of KSP/ADP/Compound 5-2b

The 3-dimensional, tertiary structure of KSP, bound with Mg^{++}-ADP and Compound 5-2b ((+)-monastrol), was determined at 2.5Å resolution with use of phases derived from a combination of molecular replacement, extensive manual rebuilding, and dynamic refinement. Two identical protein complexes were found in the asymmetric unit of the crystal and were related by a local, non-crystallographic 2-fold axis. For each, the electron density of the protein as well as those of the ligands (ADP, Mg^{++}, and Compound 5-2b) was all well defined. Compound 5-2b was seen to be of the S handedness. Residues 2–17, 272–286,and 363–368 were disordered and showed no electron densities (The N-terminal Met1 residue was processed upon expression). See Figures 1-8.

Fluorescence of Trp127 of KSP(368)-ADP -/+ Inhibitors

Materials

-2X kinesin buffer: 160 mM K-Hepes, 2 mM $MgCl_2$, 2 mM EGTA, 2 mM DTT (added fresh daily), and 100 mM KCl, pH 6.8.

-Nucleotide: nucleotide is resuspended to 200 mM in 50 mM K-Hepes (pH 6.8).

-Nucleotide is diluted 1:1 with 200 mM $MgCl_2$ to a stock concentration of 100 mM of 1:1 nucleotide:$MgCl_2$.

-Cuvette volume = 300 µl

Methods

1) Add 281 µl of 1X kinesin buffer, ± nucleotide, and H_2O (Nucleotide = none, 1 mM AMPPNP, or 1 mM ADP (final concentration)).

2) Add 18.75 µl of 4 µM stock nucleotide-free KSP(367H).

3) Add compound sequentially from DMSO stock (with all the volume of all additions ≤ 0.6 µl).

4) Measure fluorescence after each addition (starting with buffer only).

5) Example titration for Compound 8-1 with KSP(367H)ADP:
281 µl of 1X kinesin buffer + 1 mM ADP:
add 250 nM KSP (18.75 µl of 4 uM nucleotide-free stock)
add 1 nM Compound 8-1 (1 nM_f) (addition of 0.3 µl of 0.001 mM stock)
add 2 nM Compound 8-1 (3 nM_f) (addition of 0.6 µl of 0.001 mM stock)
add 4 nM Compound 8-1 (7 nM_f) (addition of 0.12 µl of 0.01 mM stock)
add 3 nM Compound 8-1 (10 nM_f) (addition of 0.09 µl of 0.01 mM stock)
add 20 nM Compound 8-1 (30 nM_f) (addition of 0.6 µl of 0.01 mM stock)
add 40 nM Compound 8-1 (70 nM_f) (addition of 0.12 µl of 0.1 mM stock)
add 30 nM Compound 8-1 (100 nM_f) (addition of 0.09 µl of 0.1 mM stock)
add 200 nM Compound 8-1 (300 nM_f) (addition of 0.6 µl of 0.1 mM stock)
add 400 nM Compound 8-1 (700 nM_f) (addition of 0.12 µl of 1 mM stock)
add 300 nM Compound 8-1 (1000 nM_f) (addition of 0.09 µl of 1 mM stock)
add 2000 nM Compound 8-1 (3000 nM_f) (addition of 0.6 µl of 1 mM stock).

6) After each addition, measure steady-state fluorescence under the following conditions:
λ_{ex} = 388 nm, λ_{em} = 342-346 nm, band width = 3 nm ex/3 nm em, wavelength increment = 0.5 nm, integration time = 2 s.

7) Repeat the same titration series:
in the absence of KSP (to determine compound-related background), and
in the absence of KSP, but in the presence of 1 µM L-tryptophan (to determine compound-related effects on the amino acid itself).

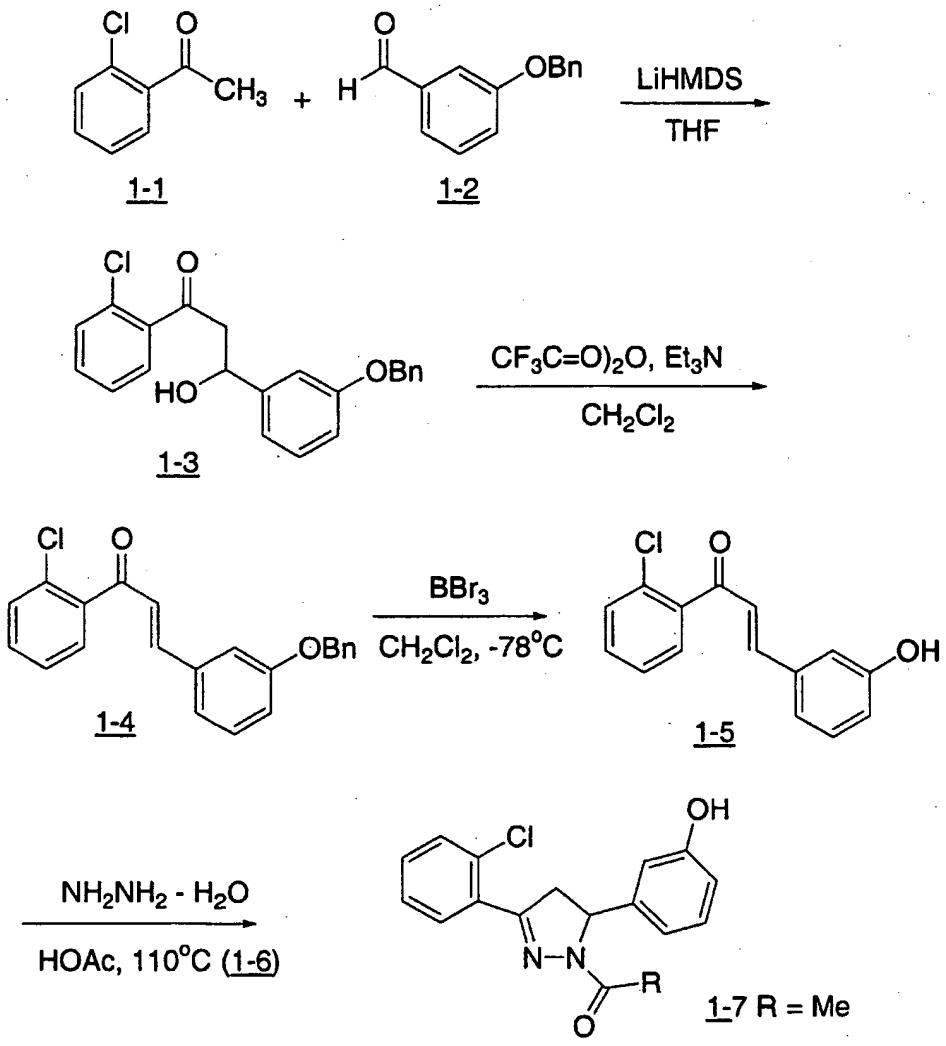
Calculations

At the peak emission wavelength for W127 in KSP(367H) (=344 nm) measure the compound emission in kinesin buffer as a function of [compound]; measure fluorescence of L-tryptophan as a function of [compound]; measure fluorescence of KSP(367H) as a function of [compound]; correct KSP(367H) fluorescence for its decrease over time (due to losses of protein to the cuvette); subtract compound emission from L-tryptophan emission; subtract compound emission from KSP(367H) emission. Calculate the fraction of fluorescence of L-tryptophan vs [compound]: (L-trp fluorescence (344 nm) at given [compound]) / (L-trp fluorescence (344 nm) at 0 cpd); calculate the fraction of fluorescence of KSP(367H) vs [compound]: (KSP fluorescence (344 nm) at given [compound]) / (KSP fluorescence (344 nm) at 0 cpd); then normalize: KSP (frcn fl) / L-trp(frcn fl) and plot vs [compound].

Results of this assay are illustrated in Figures 11-13.

Compounds that were utilized in the identification and testing of the novel KSP binding site that is disclosed herein may be prepared by the methods described below:

SCHEME 1



Step 1: 3-[3-(benzyloxy)phenyl]-1-(2-chlorophenyl)prop-2-en-1-one (1-4)

To a solution of 2'-chloroacetophenone (1-1) (1.26mL, 9.70mmol) in 40 mL of THF at –78°C was slowly added 10.7 mL (10.7mmol) of a 1M LiHMDS solution in THF. After stirring for 1h at –78°C, a solution of 2.05g (9.70mmol) of 3-benzyloxy-benzaldehyde (1-2) in

8 mL of THF was added, and stirring was continued at that temperature for an additional hour. The mixture was then dumped into a separatory funnel containing 100 mL of saturated aqueous NH_4Cl and extracted twice with 100 mL of EtOAc. The organic phases were combined, washed with 100 mL of brine, and dried over Na_2SO_4. After filtering off the drying agent, the solvent was removed on a rotary evaporator, and the residue was dissolved in 50 mL of CH_2Cl_2. After cooling to -78°C, 4 mL of triethylamine and 2 mL of trifluoroacetic anhydride were added sequentially, and the mixture was allowed to warm to rt and stir for 12h. The reaction was then dumped into a separatory funnel with 100 mL of 1M HCl, the layers were separated, and the aqueous phase extracted again with CH_2Cl_2. The organic layers were combined, washed again with 1 M HCl, washed with water, and dried over Na_2SO_4. After concentration, the crude material was purified by chromatography on silica gel with a gradient of 0 to 40% EtOAc in hexanes over 45 min to provide 1-4 as a viscous yellow oil. Data for 1-4: ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.5 – 7.0 (m, 15H) 5.1 (s, 2H) ppm.

Step 2: 1-(2-chlorophenyl)-3-(hydroxyphenyl)prop-2-en-1-one (1-5)

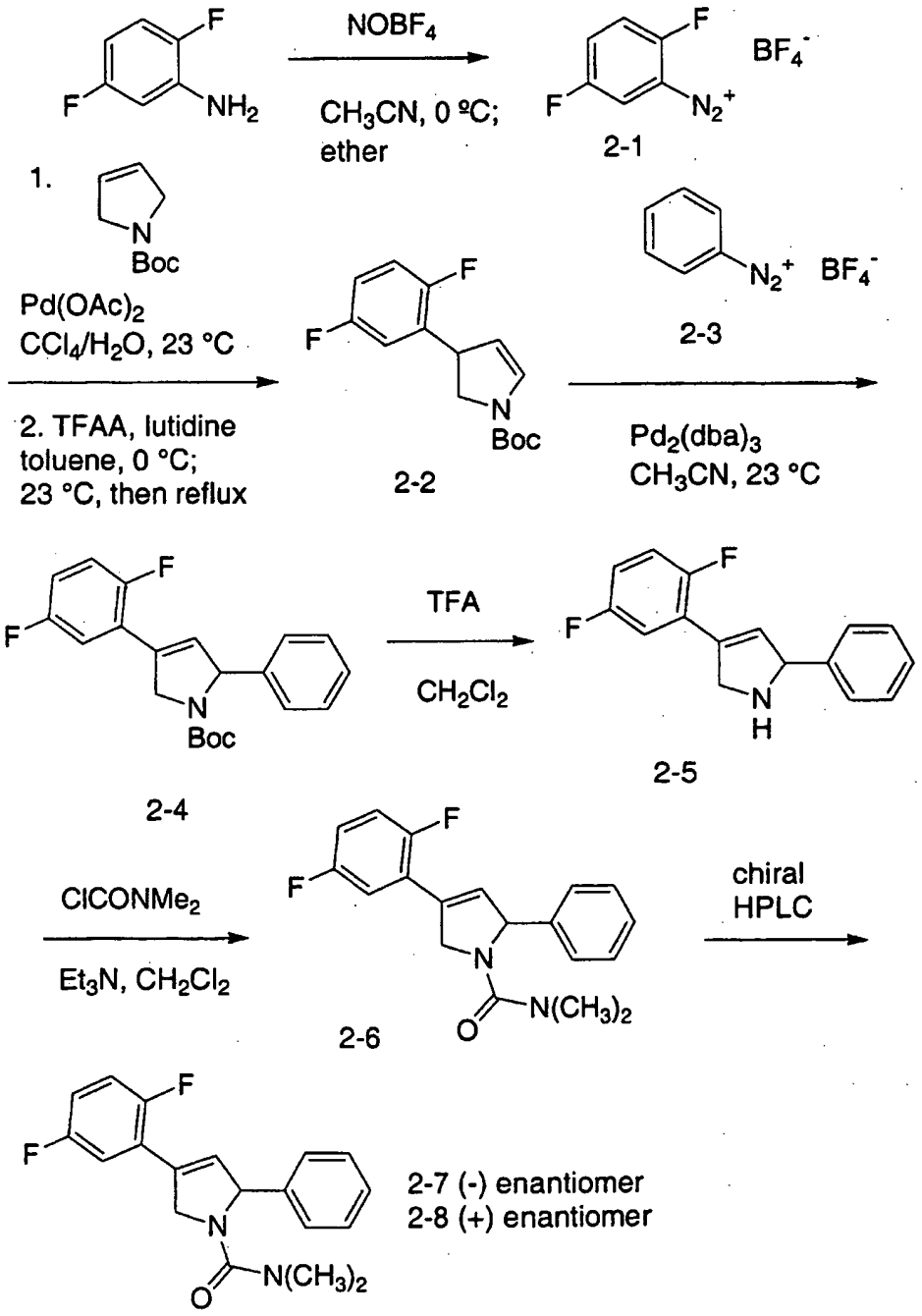
To a solution of 740 mg (2.12mmol) of 1-4 in 15 mL of CH_2Cl_2 at -78°C was added dropwise 2.75 mL (2.75mmol) of a 1M solution of BBr_3 in CH_2Cl_2. After stirring for 30 min at that temperature, 1 mL of MeOH was added, and the mixture was dumped into water, extracted twice with 50 mL of CH_2Cl_2, washed again with water, and dried over Na_2SO_4. After concentration, the residue was purified by column chromatography on silica gel with a gradient of 2 to 70% EtOAc in hexanes over 30 min to provide 1-5 as a beige solid. Data for 1-5: ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.5 – 7.3 (m, 5H), 7.25 (m, 1H), 7.2 – 7.0 (m, 3H), 6.9 (m, 1H), 5.1 (bs, 1H) ppm.

Step 3: 3-[1-acetyl-3-(2-chlorophenyl)-4,5-dihydro-1H-pyrazol-5-yl]phenol (1-7)

To a solution of 120mg (0.46mmol) of chalcone 1-5 in 4 mL of acetic acid was added 50 µL (0.93mmol) of hydrazine hydrate. The reaction was then placed in an oil bath at 110°C for 24h. After cooling to rt, the solvents were removed on a rotary evaporator, the residue was dissolved

in 50 mL of CH_2Cl_2, washed twice with aqueous $NaHCO_3$, dried over Na_2SO_4, and concentrated. The residue was then purified by column chromatography on silica gel with a gradient of 5 to 75% EtOAc in hexanes over 30 min to provide 1-7 as a fluffy white solid. Data for 1-7: ^{1}HNMR (500 MHz, $CDCl_3$) δ 7.75 (m, 1H), 7.45 (m 1H), 7.4 – 7.3 (m, 2H), 7.2 (m, 1H), 6.8 (d, 1H), 6.7 (m, 2H), 5.5 (m, 1H), 3.9 (m, 1H), 3.3 (m, 1H), 2.4 (s, 3H) ppm. HRMS (ES) calc'd M + H for $C_{17}H_{15}ClN_2O_2$: 315.0895. Found: 315.0904.

SCHEME 2


NOBF4
CH3CN, 0 ºC;
ether
BF4-
2-1
1.
N
Boc
Pd(OAc)2
CCl4/H2O, 23 °C
2. TFAA, lutidine
toluene, 0 °C;
23 °C, then reflux
2-2
N2+ BF4-
2-3
Pd2(dba)3
CH3CN, 23 °C
TFA
CH2Cl2
2-4
2-5
ClCONMe2
Et3N, CH2Cl2
2-6
chiral
HPLC
2-7 (-) enantiomer
2-8 (+) enantiomer

Step 1: 2,5-difluorobenzenediazonium tetrafluoroborate (2-1)

Nitrosonium tetrafluoroborate (905 mg, 7.75 mmol, 1.00 equiv) was added to a solution of 2,5-difluoroaniline (0.780 mL, 7.75 mmol, 1 equiv) in acetonitrile (50 mL) at 0°C. The resulting mixture was stirred for 1 h, then diluted with ethyl ether (150 mL). The precipitate was filtered and air-dried to give 2,5-difluorobenzenediazonium tetrafluoroborate (2-1) as a tan solid. ^{1}H NMR (300 MHz, CD_3OD) δ 8.54 (m, 1H), 8.24 (m, 1H), 7.95 (m, 1H).

Step 2: tert-butyl 3-(2,5-difluorophenyl)-2,3-dihydro-1H-pyrrole-1-carboxylate (2-2)

Palladium(II) acetate (67 mg, 0.30 mmol, 0.020 equiv) was added to a vigourously stirred, deoxygenated mixture of tert-butyl 2,5-dihydro-1H-pyrrole-1-carboxylate (2.59 mL, 15.0 mmol, 1 equiv) and 2,5-difluorobenzenediazonium tetrafluoroborate (2-1, 3.42 g, 15.0 mmol, 1.00 equiv) in water and carbon tetrachloride (1:1, 150 mL) at 23°C, and the resulting mixture was stirred for 20 h. The reaction mixture was concentrated, and the residue partitioned between ethyl acetate (300 mL) and saturated aqueous sodium bicarbonate solution (75 mL). The organic layer was washed with brine, then dried over sodium sulfate and concentrated. The residue was dissolved in toluene (200 mL), and the resulting solution concentrated *in vacuo* to facilitate azeotropic removal of residual water. 2,6-Lutidine (3.50 mL, 30.0 mmol, 2.00 equiv) and trifluoroacetic anhydride (1.48 mL, 10.5 mmol, 0.700 equiv) were then sequentially added to a solution of the residue in toluene (100 mL) at -10°C. The resulting mixture was allowed to warm to 10 °C over 16 h, then heated at reflux for 1 h. The reaction mixture was allowed to cool to 23°C, then concentrated. The residue was partitioned between ethyl acetate (300 mL) and saturated aqueous sodium bicarbonate solution (150 mL). The organic layer was dried over sodium sulfate and concentrated. The residue was purified by flash column chromatography (hexanes initially, grading to 20% EtOAc in hexanes) to give tert-butyl 3-(2,5-difluorophenyl)-2,3-dihydro-1H-pyrrole-1-carboxylate (2-2) as a red oil. ^{1}H NMR (500 MHz, $CDCl_3$) major rotamer: δ 7.03-6.84 (m, 3H), 6.70 (br s, 1H), 5.01 (br s, 1H), 4.42 (m, 1H), 4.13 (m, 1H), 3.60 (m, 1H), 1.50 (s, 9H).

Step 3: tert-butyl 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxylate (2-4)

Tris(dibenzylideneacetone)dipalladium(0) (59 mg, 064 mmol, 0.020 equiv) was added to a deoxygenated mixture of tert-butyl 3-(2,5-difluorophenyl)-2,3-dihydro-1H-pyrrole-1-carboxylate (2-2, 900 mg, 3.20 mmol, 1 equiv), benzenediazonium tetrafluoroborate (1-3, prepared by the method described above for 2-3, 614 mg, 3.20 mmol, 1.00 equiv), and sodium acetate trihydrate (1.32 g, 9.60 mmol, 3.00 equiv) in acetonitrile (70 mL) at 23°C. The reaction mixture was stirred for 16 h, then partitioned between saturated aqueous sodium bicarbonate solution and ethyl acetate (2 x 70 mL). The combined organic layers were dried over sodium sulfate and concentrated. The residue was purified by flash column chromatography (hexanes initially, grading to 40% hexanes in EtOAc) to provide tert-butyl 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxylate (2-4) as an orange oil. LRMS *m/z* (M+H-CH_3) 343.0 found, 343.1 required.

Step 4: 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole (2-5)

Trifluoroacetic acid (20 mL) was added to a solution of tert-butyl 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxylate (2-4, 700 mg, 1.96 mmol, 1 equiv) in dichloromethane (50 mL) at 23 °C, and the resulting mixture was stirred for 30 min, then concentrated to give 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole (2-5) as a TFA salt (brown oil). LRMS *m/z* (M+H) 258.1 found, 258.1 required.

Step 5: 4-(2,5-difluorophenyl)-N,N-dimethyl-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxamide (2-6)

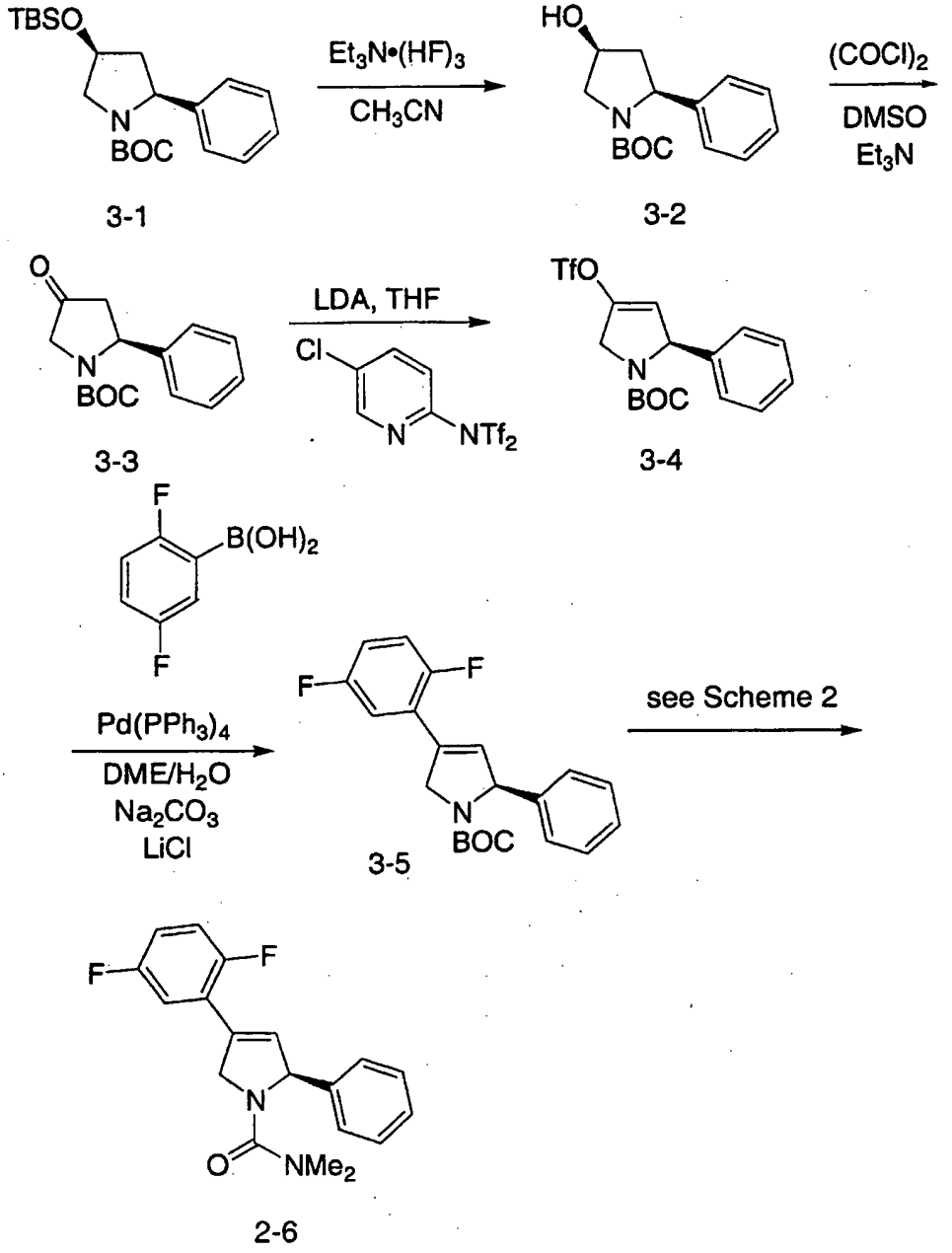
Triethylamine (1.37 mL, 9.79 mmol, 5.00 equiv) and dimethylcarbamoyl chloride (0.180 mL, 1.96 mmol, 1.00 equiv) were added to a solution of 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole (2-5, 1.96 mmol) in dichloromethane (50 mL) at 23°C, and the resulting mixture was stirred for 2 h, then concentrated. The residue was partitioned between saturated aqueous sodium bicarbonate solution (75 ml) and ethyl acetate (100 mL). The organic layer was dried over sodium sulfate and concentrated. The residue was purified by reverse-phase LC (H_2O/CH_3CN

gradient w/ 0.1 % TFA present) to provide 4-(2,5-difluorophenyl)-N,N-dimethyl-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxamide (2-6) as an off-white solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.35-7.29 (m, 4H), 7.25 (m, 1H), 7.05 (m, 1H), 7.00 (m, 1H), 6.96 (m, 1H), 6.40 (br s, 1H), 6.13 (m, 1H), 4.88 (ddd, 1H, J = 13.7, 5.6, 2.0 Hz), 4.52 (d, 1H, J = 13.7 Hz), 2.88 (s, 6H). LRMS *m/z* (M+H) 329.1 found, 329.1 required.

Step 6: Enantiomers of 4-(2,5-difluorophenyl)-N,N-dimethyl-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxamide (2-7 and 2-8)

Resolution of enantiomers of racemic 4-(2,5-difluorophenyl)-N,N-dimethyl-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxamide (2-6) by chiral normal-phase HPLC (Chiralcel OD column: 0.1 % diethylamine in 40% ethanol in hexanes) provided in order of elution 2-7 (-) and 2-8 (+).

SCHEME 3


TBSO
N
BOC
3-1
$Et_3N•(HF)_3$
CH_3CN
HO
N
BOC
3-2
$(COCl)_2$
DMSO
Et_3N
O
N
BOC
3-3
LDA, THF
Cl
N
NTf_2
TfO
N
BOC
3-4
F
$B(OH)_2$
F
$Pd(PPh_3)_4$
DME/H_2O
Na_2CO_3
LiCl
F
F
N
BOC
3-5
see Scheme 2
F
F
N
O
NMe_2
2-6

5

Step 1: (2S,4S)-tert-Butyl 4-hydroxy-2-phenylpyrrolidine-1-carboxylate (3-2)

To a flame dried flask equipped with stir bar was added tert-butyl (2S,4S)-4-{[tert-butyl(dimethyl)silyl]oxy}-2-phenylpyrrolidine-1-carboxylate (3-1, prepared from (*S*)-(-)-4-chloro-3-hydroxybutyronotrile by the method of Maeda, *et al Synlett* **2001**, 1808-1810, 7.8 g, 20.7 mmol) and anhydrous acetonitrile (20.0 mL). The resulting solution was treated with triethylamine trihydrofluoride (10.1 mL, 62.0 mmol) while stirring under N_2. The reaction stirred 12 h at 40 °C. The reaction was then diluted with EtOAc (100 mL) and poured into 5% aq. $NaHCO_3$. Following cessation of gas evolution, the organic layer was washed three addition times with 5% aq. $NaHCO_3$. The organic layer was dried over magnesium sulfate, filtered and concentrated to provide crude product. Recrystallization was effected from EtOAc/hexanes to provide (2S,4S)-tert-butyl 4-hydroxy-2-phenylpyrrolidine-1-carboxylate (3-2) as a white crystalline solid. ^{1}H NMR (300 MHz, $CDCl_3$) rotamers δ 7.38-7.18 (m, 5H), 4.90 (m, 1H), 4.42 (m, 1H), 3.88 (m, 1H), 3.56 (dd, J = 11.5, 4.0 Hz, 1H), 2.60 (m, 1H), 2.03 (m, 1H), 1.50 and 1.20 (br s, 9H); MS 208.0 found, 208.1 (M – $C(CH_3)_3$) required.

Step 2: (2S)-tert-butyl 4-oxo-2-phenylpyrrolidine-1-carboxylate (3–3)

To a flame dried flask equipped with stir bar was added 150 mL anhydrous dichloromethane which was cooled to –78 °C. Oxalyl chloride (3.8 mL, 44 mmol) and DMSO (4.8 mL, 61 mmol) were added sequentially and the reaction stirred for 10 min. (2S,4S)-tert-butyl 4-hydroxy-2-phenylpyrrolidine-1-carboxylate (3-2, 2.28 g, 8.73 mmol) in 10 mL anhydrous dichloromethane was added dropwise and stirred 1 h at –78°C. Triethylamine (12 mL, 87mmol) was added and the reaction was warmed to 0°C over 1 h. Upon completion, the reaction was washed with 5% $NaHCO_3$, brine and dried over $MgSO_4$. The organic layer was concentrated to provide crude (2S)-tert-butyl 4-oxo-2-phenylpyrrolidine-1-carboxylate (3–3). Recrystallization was effected with EtOAc/hexanes. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35 (m, 3H), 7.17 (m, 2H), 5.38 (m, 1H), 4.08 (d, J = 19.5 Hz, 1H), 3.90 (d, J = 19.3 Hz, 1H), 3.13 (dd, J = 18.8, 9.8 Hz,

1H), 2.58 (dd, J = 18.6, 2.4 Hz, 1H), 1.40 (br s, 9H); MS 206.0 found, 206.1 (M – $C(CH_3)_3$) required.

Step 3: (2S)-tert-butyl 2-phenyl-4-{[(trifluoromethyl)sulfonyl]oxy}-2,5-dihydro-1H-pyrrole-1-carboxylate (3–4)

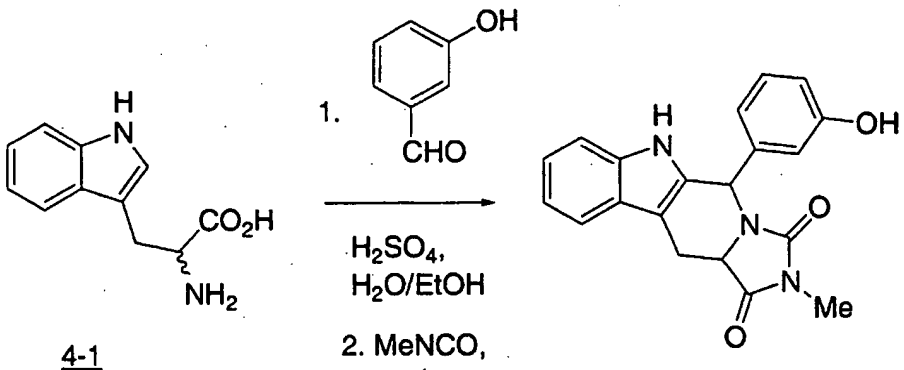
To a flame dried flask equipped with stir bar was added ketone (2S)-tert-butyl 4-oxo-2-phenylpyrrolidine-1-carboxylate (3–3, 0.16 g, 0.62 mmol) and anhydrous THF (2 mL). The resulting solution was cooled to –78 °C, and treated dropwise with lithium hexamethyldisilylamide (LHMDS, 0.68 mL, 1M in THF, 0.68 mmoL). The reaction stirred 1 h at –78 °C, and N-(5-chloropyridin-2-yl)-1,1,1-trifluoro-N-[(trifluoromethyl)sulfonyl]-methanesulfonamide (0.27 g, 068 mmol) was added neat in one portion. The reaction was allowed to warm to 0 °C and stirred 4 hours total. The reaction was diluted with Et2O (10mL) and washed successively with H_2O (10mL) and brine (10 mL). The organic layer was dried over $MgSO_4$, filtered and concentrated. The crude residue was purified by flash column choromatography (0-20% EtOAc/hexanes gradient, 15 min) to provide (2S)-tert-butyl 2-phenyl-4-{[(trifluoromethyl)sulfonyl]oxy}-2,5-dihydro-1H-pyrrole-1-carboxylate (3-4). ^{1}H NMR (300 MHz, $CDCl_3$) major rotamer: δ 7.30 (m, 5H), 5.72 (m, 1H), 5.48 (m, 1H), 4.42 (m, 2H), 1.18 (s, 9H); MS 379.0 found 379.1 (M – CH_3) required.

Step 4: (2S)-4-(2,5-difluorophenyl)-2-phenyl-N,N-dimethyl-2,5-dihydro-1H-pyrrole-1-carboxamide (3-5)

To a flame dried flask equipped with stir bar was added (2S)-tert-butyl 2-phenyl-4-{[(trifluoromethyl)sulfonyl]oxy}-2,5-dihydro-1H-pyrrole-1-carboxylate (3–4, 0.250 g, 0.636 mmol), 2,5-difluorophenyl boronic acid (0.251 g, 1.59 mmol), Na_2CO_3 (0.202 g, 1.91 mmol), and LiCl (0.081 g, 1.91 mmol). The solids were dissolved in 20 mL 4:1 DME/H_2O and degassed with nitrogen. $Pd(PPh_3)_4$ (0.037 g, 0.032 mmol) was added and the reaction was sealed under nitrogen and heated to 90 °C for 2 h. Upon completion, the reaction was partitioned between 5% aq. $NaHCO_3$ and EtOAc (3 x 50 mL), and the combined organic layers were dried over $MgSO_4$. Following filtration, the organic layer was concentrated and

purified via flash column chromatography (SiO_2, 0-20% EtOAc/hexanes gradient) to provide (2S)-tert-butyl 4-(2,5-difluorophenyl)-2-phenyl-2,5-dihydro-1H-pyrrole-1-carboxylate (3-5). Further transformations followed those described in Scheme 1 to provide the instant compound 2-6.

SCHEME 4



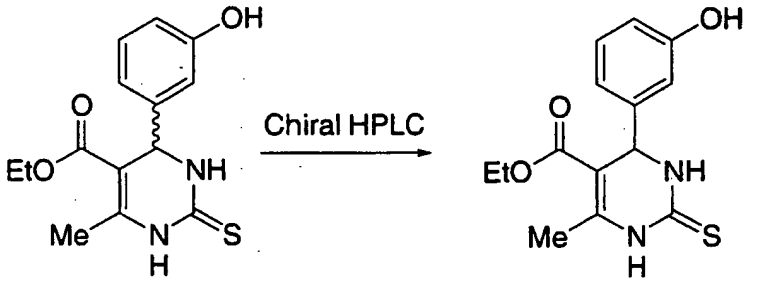
4-2a (Trans)
4-2b (Cis)

Trans-1H-Imidazo[1',5':1,6]pyrido[3,4-b]indole-1,3(2H)-dione,5,6,11,11a-tetrahydro-2-methyl-5-(3-hydroxyphenyl) (4-2a)

To a mixture of DL-tryptophan (1.5 g, 7.44 mmol), 3-hydroxybenzaldehyde (0.90, 7.44 mmol) in EtOH (3 mL) was added aq. H_2SO_4 (14.9 mL of a 0.5 M solution). The reaction was heated to 50 C for 12 h. The reaction mixture was partly concentrated to remove EtOH and resuspended in H_2O (5 mL). The precipitate was collected by filtration and dried in vacuo. The portion of this solid residue (0.14 g, 0.47 mmol) was dissolved in acetone (3 mL) and treated with methyl isocyanate. The reaction mixture was heated at 150 C in a sealed vessel for 15 min in a microwave reactor. The reaction was cooled to r.t. and concentrated. The residue was absorbed onto silica gel then purified on an ISCO automated system affixed with a Biotage flash 40(s) cartridge eluting with 0-100% EtOAc in hexane at 20 mL/min over 30 min to afford a mixture of 4-2a/4-2b Trituration of this mixture with diethyl

ether provided pure 4-2a. Data for 4-2a: ^{1}HNMR (600 MHz, CD_3OD) δ 7.52 (d, J = 8 hz, 1H), 7.27 (d, J = 8 hz, 1H), 7.18 (m, 1H), 7.12 (m, 1H), 7.07 (m, 1H), 6.84 (m, 1H), 6.74 (m, 2H), 6.24 (s, 1H), 4.44 (m, 1H), 3.43 (m, 1H), 3.01 (s, 3H), 2.88 (m, 1H) ppm. HRMS Calcd (M+1) 348.1270; found 348.1343.

SCHEME 5



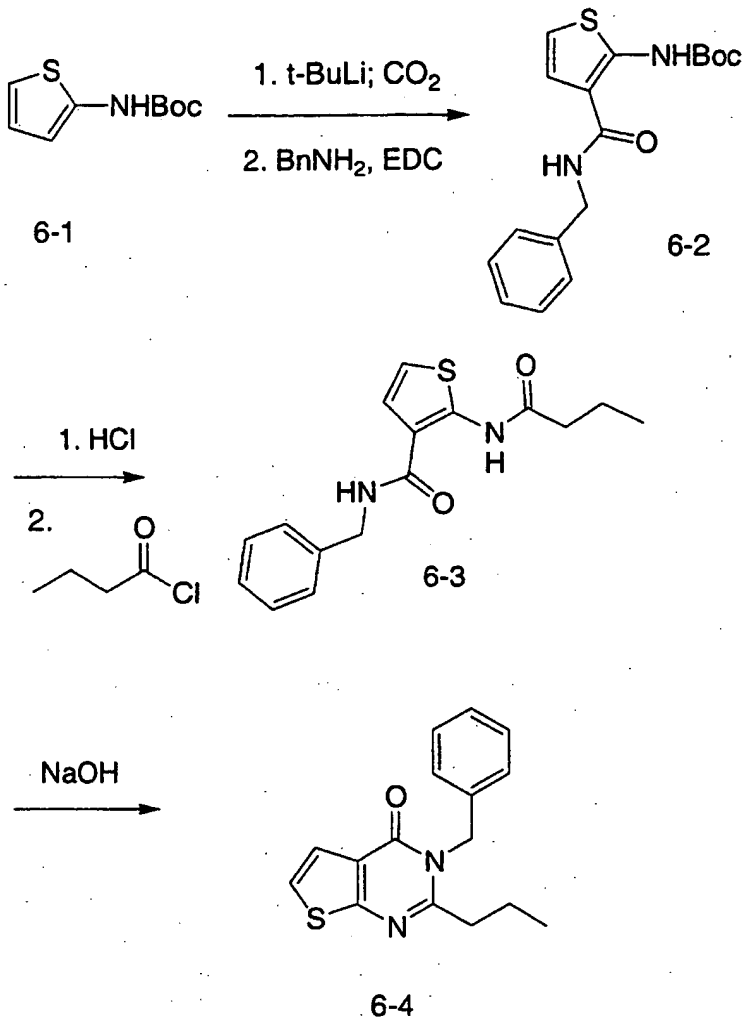
5-1

5-2a (-)-enantiomer
5-2b (+)-enantiomer

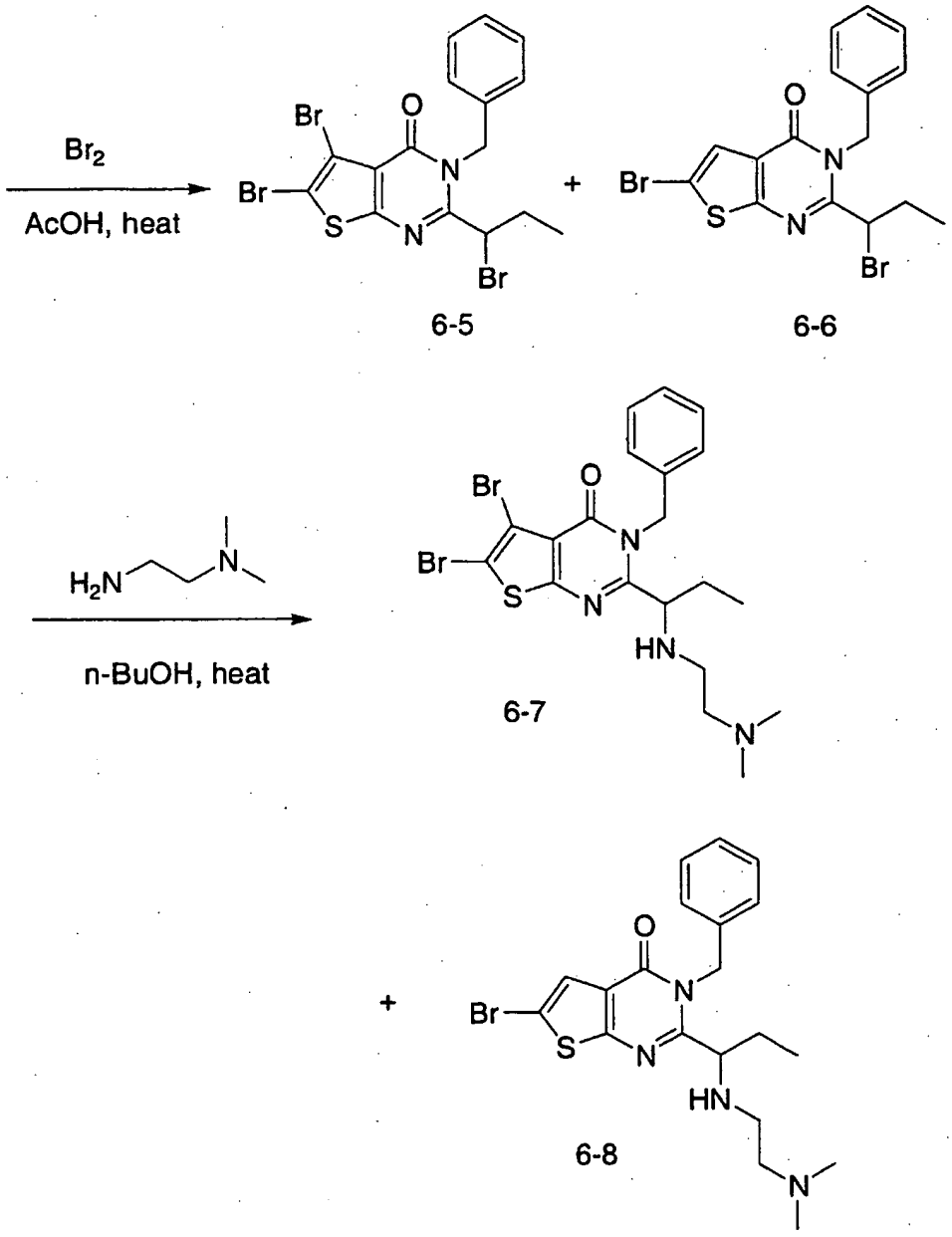
(-)4-(3-Hydroxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro-4H-pyrimidin-5-carboxylic acid ethyl ester (5-2a) and (+)-4-(3-Hydroxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro-4H-pyrimidin-5-carboxylic acid ethyl ester (5-2b)

Racemic monastrol (50 mg, Tocris) was resolved by chiral HPLC (Chiralpak AD column 5 x 50 cm; 20% EtOH/80% (hexanes + 0.1% diethylamine); flow = 60 mL/min) to yield (-)-enantiomer 1-2A (R_T=57.0 min) and (+)-enantiomer 5-2 B (R_T = 71.2 min). Enantiomer 5-2B was crystallized from hexanes to yield a yellow solid.

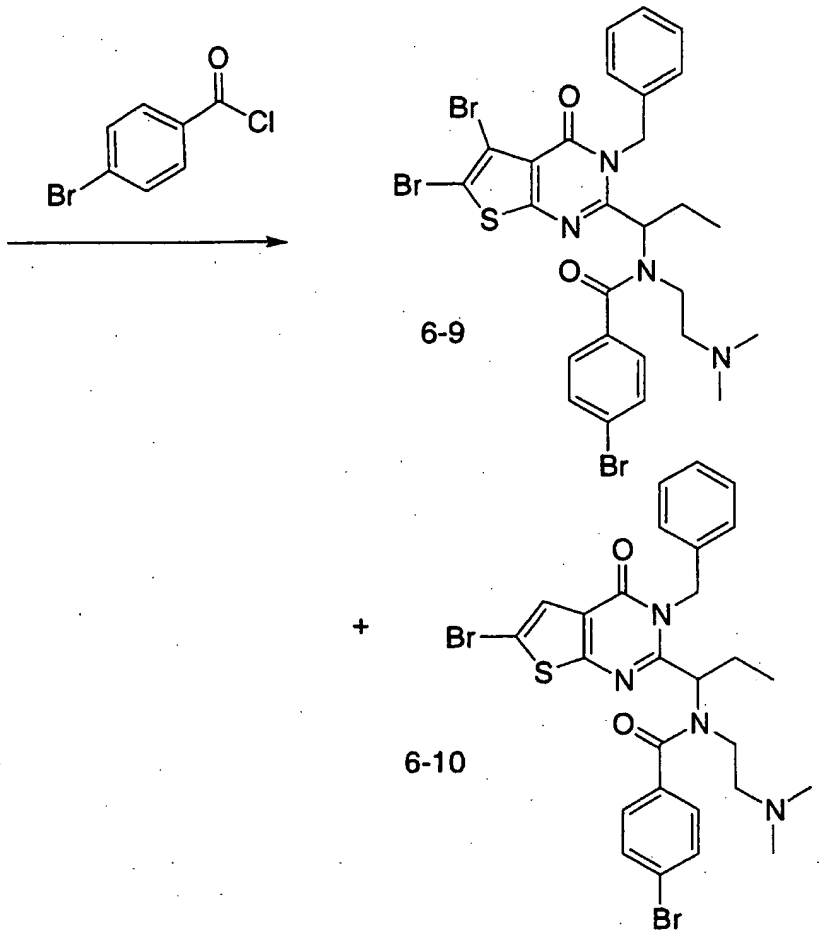
SCHEME 6


S
NHBoc
1. t-BuLi; CO2
2. BnNH2, EDC
6-1
S
NHBoc
O
HN
6-2
1. HCl
2.
O
Cl
S
O
N
H
HN
O
6-3
NaOH
O
N
S
N
6-4

SCHEME 6 (continued)



SCHEME 6 (continued)



tert-Butyl 3-[(benzylamino)carbonyl]thien-2-ylcarbamate (6-2)

A solution of tert-butyllithium in pentane (1.7 M, 42.5 mL, 72.3 mmol, 2.40 equiv) was added to a solution of tert-butyl thien-2-ylcarbamate (6-1, 6.00 g, 30.1 mmol, 1 equiv) in THF (300 mL) at –78 °C. The reaction mixture was stirred for 45 min, then solid CO_2 (approximately 20 g) was added and the resulting mixture was warmed to 0 °C and stirred for 30 minutes. The reaction mixture was partitioned between aqueous 1 N hydrochloric acid solution and ethyl acetate (2 x 150 mL). The combined organic layers were dried over sodium sulfate and concentrated. The residue

was purified by flash column chromatography (hexanes initially, grading to 100% ethyl acetate), and the polar fractions were concentrated. A solution of the residue, benzylamine (6.61 g, 61.7 mmol, 2.05 equiv), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (5.91 g, 30.8 mmol, 1.02 equiv), 1-hydroxy-7-azabenzotriazole (4.19 g, 30.8 mmol, 1.02 equiv), and triethylamine (8.59 mL, 61.7 mmol, 2.05 equiv) in DMF (100 mL) was stirred at 55°C for 24 h. The reaction mixture was concentrated, and the residue was partitioned between saturated aqueous sodium bicarbonate solution and ethyl acetate (3 x 100 mL). The combined organic layers were dried over sodium sulfate and concentrated. The residue was purified by flash column (hexanes initially, grading to 100% ethyl acetate) to give tert-butyl 3-[(benzylamino)carbonyl]thien-2-ylcarbamate (6-2) as a colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.37 (m, 5H), 6.87 (d, 1H, J = 5.8 Hz), 6.69 (d, 1H, J = 5.8 Hz), 6.13 (s, 1H), 4.61 (d, 2H, J = 5.5 Hz), 1.52 (s, 9H).

N-benzyl-2-(butyrylamino)thiophene-3-carboxamide (6-3)

A solution of tert-butyl 3-[(benzylamino)carbonyl]thien-2-ylcarbamate (6-2, 500 mg, 1.50 mmol, 1 equiv) was saturated with HCl gas at 0 °C, and the resulting solution was stirred at 0 °C for 1 h, then allowed to warm to 23 °C and stirred for 1 h. The reaction mixture was concentrated and the residue was dissolved in pyridine (10 mL). The resulting solution was cooled to 0 °C, and butyryl chloride (420 µL, 4.04 mmol, 2.69 equiv) was added in three equal portions over 1 h. The reaction mixture was partitioned between aqueous sodium bicarbonate solution and ethyl acetate (50 mL). The organic layer was dried over sodium sulfate and concentrated. The residue was purified by flash column (hexanes initially, grading to 100% ethyl acetate) to give N-benzyl-2-(butyrylamino)thiophene-3-carboxamide (6-3) as an off-white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36 (m, 5H), 6.92 (d, 1H, J = 6.1 Hz), 6.76 (d, 1H, J = 5.8 Hz), 6.23 (s, 1H), 4.62 (d, 2H, J = 5.8 Hz), 2.47 (t, 2H, J = 7.3 Hz), 1.80 (sextet, 2H, J = 7.3 Hz), 1.01 (t, 3H, J = 7.3 Hz).

3-benzyl-2-propylthieno[2,3-d]pyrimidin-4(3H)-one (6-4)

A mixture of N-benzyl-2-(butyrylamino)thiophene-3-carboxamide (6-3, 230 mg, 0.76 mmol, 1 equiv) and sodium hydroxide (3 mg, 0.08 mmol, 0.1 equiv) in ethylene glycol (5 mL) was heated at 130 °C for 5 h. The reaction mixture was allowed to cool, then partitioned between a half-saturated aqueous sodium chloride solution and ethyl acetate (2 x 75 mL). The combined organic layers were dried over sodium sulfate and concentrated. The residue was purified by flash column (hexanes initially, grading to 100% ethyl acetate) to provide 3-benzyl-2-propylthieno[2,3-d]pyrimidin-4(3H)-one (6-4) as a colorless oil which solidified upon standing. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.48 (d, 1H, J = 5.8 Hz), 7.31 (m, 3H), 7.19 (d, 1H, J = 5.8 Hz), 7.17 (d, 2H, J = 7.9 Hz), 5.42 (s, 2H), 2.72 (t, 2H, J = 7.6 Hz), 1.78 (sextet, 2H, J = 7.6 Hz), 0.97 (t, 3H, J = 7.3 Hz).

3-benzyl-5,6-dibromo-2-(1-bromopropyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-5) and 3-benzyl-6-bromo-2-(1-bromopropyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-6)

A solution of 3-benzyl-2-propylthieno[2,3-d]pyrimidin-4(3H)-one (6-4, 100 mg, 0.35 mmol, 1 equiv), potassium acetate (207 mg, 2.1 mmol, 6 equiv) and bromine (338 mg, 2.1 mmol, 6 equiv) in acetic acid (2 mL) was heated at 100°C for 3 hr. The reaction was concentrated, and the residue was purified by flash chromatography. Elution with 30 % hexanes/EtOAc gave 3-benzyl-5,6-dibromo-2-(1-bromopropyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-5) as a colorless solid. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.30 (m, 1H), 7.14 (d, J = 7.3 Hz, 2H), 6.19 (d, J = 16.3 Hz, 1H), 4.87 (d, J = 16.3 Hz, 1H), 4.62 (t, J = 7.3 Hz, 1H), 2.35 (m, 1H), 2.18 (m, J = 1H), 0.72 (t, J = 7.3 Hz, 3H). Further elution with the same eluant gave 3-benzyl-6-bromo-2-(1-bromopropyl)thieno[2,3-d]pyrimidin-4(3H)-one (2-6) as a colorless gum. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (s, 1H), 7.34 (m, 2H), 7.29 (m, 1H), 7.12 (d, J = 7.3 Hz, 2H), 6.21 (d, J = 16.3 Hz, 1 H), 4.88 (d, J = 16.3 Hz, 1H), 4.62 (t, J = 7.2 Hz, 1H), 2.37 (m, 1H), 2.18 (m, 1H), 0.72 (t, J = 7.3 Hz, 3H).

3-benzyl-5,6-dibromo-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-7)

A solution of 3-benzyl-5,6-dibromo-2-(1-bromopropyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-5, 35 mg, 0.066 mmol, 1 equiv) and N,N-dimethylethylenediamine (17 mg, 0.198 mmol, 3 equiv) in ethanol (5mL) was heated at reflux for 18 h. The reaction was concentrated, and the residue was partitioned between EtOAc and brine. The organic layer was dried ($MgSO_4$) and concentrated to provide 3-benzyl-5,6-dibromo-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno-[2,3-d]pyrimidin-4(3H)-one (6-7) as a yellow gum. MS(M+1) = 526.8.

3-benzyl-6-bromo-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-8)

A solution of 3-benzyl-6-bromo-2-(1-bromopropyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-6, 35 mg, 0.079 mmol, 1 equiv) and N,N-dimethylethylenediamine (21 mg, 0.237 mmol, 3 equiv) in ethanol (5mL) was heated at reflux for 18 h. The reaction was concentrated, and the residue was partitioned between EtOAc and brine. The organic layer was dried ($MgSO_4$) and concentrated to provide 3-benzyl-6-bromo-2-(1-{[2-(dimethylamino)ethyl]amino}-propyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-8) as a yellow gum. MS(M+1) = 449.9.

N-[1-(3-benzyl-5,6-dibromo-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidin-2-yl)propyl]-4-bromo-N-[2-(dimethylamino)ethyl]benzamide (6-9)

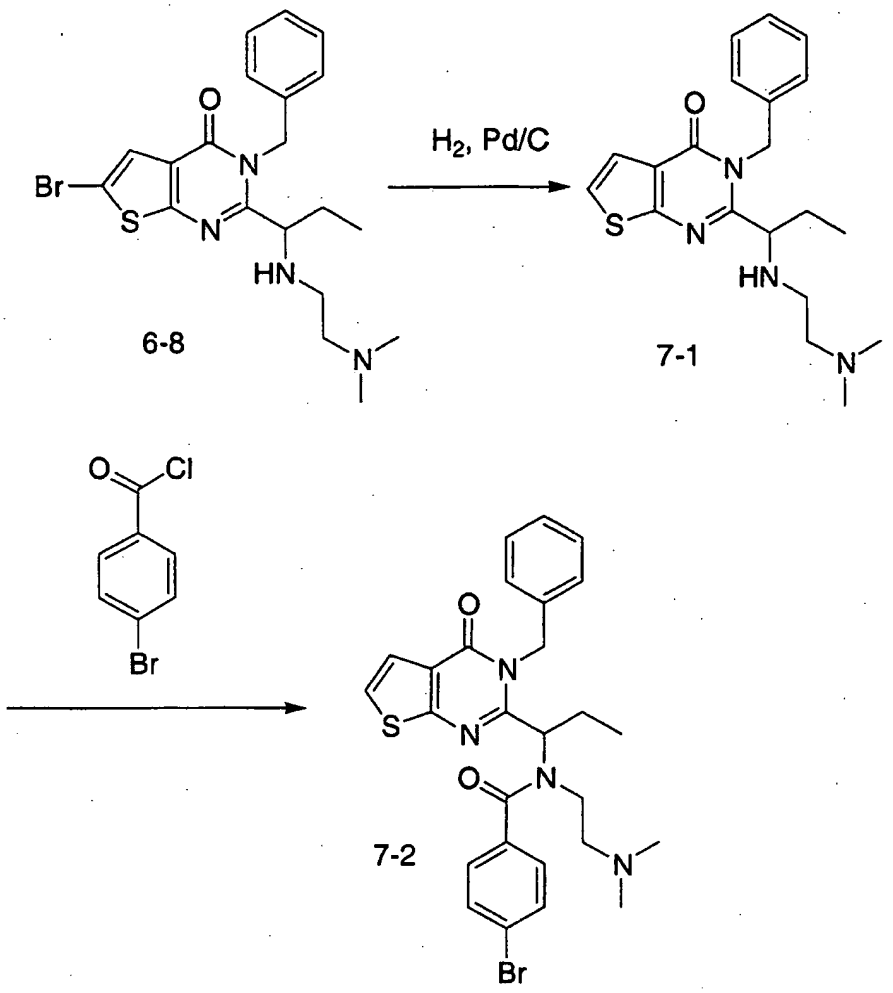
A solution of 4-bromobenzoyl chloride (19 mg, 0.085 mmol, 1 equiv) in dichloromethane (1 mL) was added to a solution of 3-benzyl-5,6-dibromo-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-8, 45 mg, 0.085 mmol, 1 equiv) and N,N-diisopropylethylamine (11 mg, 0.085 mmol, 1 equiv) in dichloromethane (5 mL), and the resulting reaction mixture was stirred under ambient conditions for 1 h. The reaction mixture was washed with saturated aqueous $NaHCO_3$ solution, then brine, and dried ($MgSO_4$) and concentrated. The residue was purified by reverse-phase LC (H_2O/CH_3CN gradient w/ 0.1 % TFA present) to provide N-[1-(3-benzyl-5,6-dibromo-4-oxo-3,4-dihydrothieno[2,3-

d]pyrimidin-2-yl)propyl]-4-bromo-N-[2-(dimethylamino)ethyl]benzamide (6-9) as a colorless foam. MS(M+1) = 708.9

N-[1-(3-benzyl-6-bromo-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidin-2-yl)propyl]-4-bromo-N-[2-(dimethylamino)ethyl]benzamide (6-10)

A solution of 4-bromobenzoyl chloride (19 mg, 0.085 mmol, 1 equiv) in dichloromethane (1 mL) was added to a solution of 3-benzyl-6-bromo-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one (6-9, 38 mg, 0.085 mmol, 1 equiv) and N,N-diisopropylethylamine (11 mg, 0.085 mmol, 1 equiv) in dichloromethane (5 mL), and the resulting reaction mixture was stirred under ambient conditions for 1 h. The reaction mixture was washed with saturated aqueous $NaHCO_3$ solution, and brine, then dried ($MgSO_4$) and concentrated. The residue was purified by reverse-phase LC (H_2O/CH_3CN gradient w/ 0.1 % TFA present) to provide N-[1-(3-benzyl-6-bromo-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidin-2-yl)propyl]-4-bromo-N-[2-(dimethylamino)ethyl]benzamide (6-10) as a colorless foam. ^1H NMR (500 MHz, $CDCl_3$) δ 7.55 (m, 3H), 7.31 (m, 5H), 7.14 (m, 2H), 6.04 (d, J = 15.4 Hz, 1H), 5.92 (m, 1H), 5.12 (d, J = 15.4 Hz, 1H), 3.37 (m, 2H), 2.05 (m, 4 H), 1.83 (m, 6H), 0.65 (m, 3H).

SCHEME 7



3-benzyl-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one (7-1)

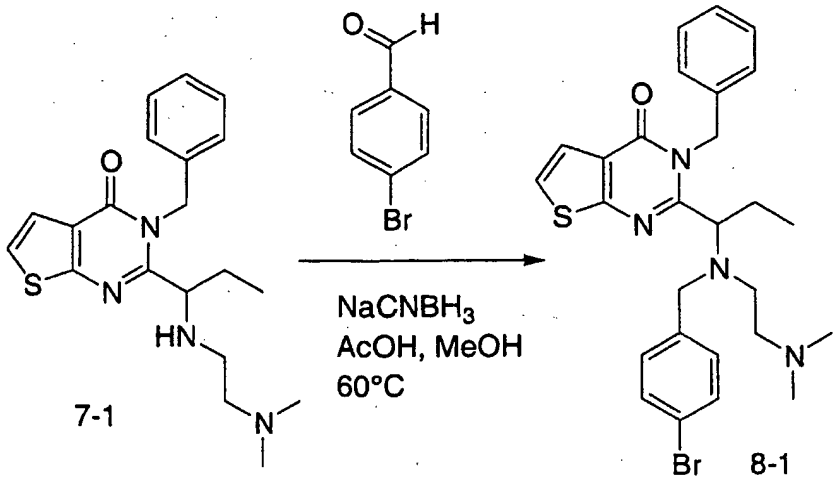
A mixture of 3-benzyl-6-bromo-2-(1-{[2-(dimethylamino)ethyl]-amino}propyl)-thieno[2,3-d]pyrimidin-4(3H)-one (6-8,17 mg, 0.38 mmol, 1 equiv) and 10 % Pd/C in ethyl acetate (5 mL) was hydrogenated at 1 atm. for 3 h. The mixture was filtered and the filtrate concentrated to provide 3-benzyl-2-(1-{[2-

(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one (7-1) as a pale yellow gum. MS(M+1) = 371.1.

N-[1-(3-benzyl-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidin-2-yl)propyl]-4-bromo-N-[2-(dimethylamino)ethyl]benzamide (7-2)

A solution of 4-bromobenzoyl chloride (8 mg, 0.035 mmol, 1 equiv) in dichloromethane (1 mL) was added to a solution of 3-benzyl-2-(1-{[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-d]pyrimidin-4(3H)-one (7-1, 13 mg, 0.035 mmol, 1 equiv) and N,N-diisopropylethylamine (5 mg, 0.035 mmol, 1 equiv) in dichloromethane (1 mL), and the resulting mixture was stirred under ambient conditions for 1 h. The reaction mixture was washed with saturated aqueous $NaHCO_3$ solution, and brine, then dried ($MgSO_4$) and concentrated. The residue was purified by flash chromatography. Elution with CH_2Cl_2 to 5 % NH_3-EtOH/CH_2Cl_2 gave N-[1-(3-benzyl-4-oxo-3,4-dihydrothieno[2,3-d]pyrimidin-2-yl)propyl]-4-bromo-N-[2-(dimethylamino)ethyl]benzamide (7-2) as an off-white foam. ^1H NMR (500 MHz, $CDCl_3$) δ 7.31 (m, 5H), 7.14 (m, 2H), 6.09 (d, J = 15.6 Hz, 1H), 5.94 (m, 1H), 5.10 (d, J = 15.6 Hz, 1H), 3.40 (m, 2H), 2.11 (m, 1H), 2.03 (m, 2H), 1.87 (m, 1H), 1.79 (s, 6H), 0.66 (t, J = 6.6 Hz, 3H).

SCHEME 8



3-benzyl-2-(1-{(4-bromobenzyl)[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-*d*]pyrimidin-4(3*H*)-one(8-1)

A solution of 3-benzyl-2-(1-{[2-(dimethylamino)ethyl]amino}-propyl)thieno[2,3-*d*]pyrimidin-4(3*H*)-one(7-1, 175 mg, 0.47 mmol, 1 equiv) and 4-bromobenzaldehyde (174 mg, 0.94 mmol, 2 equiv) in methanol (20 mL) was treated with a solution of sodium cyanoborohydride in tetrahydrofuran (1 M, 0.94 mL, 0.94 mmol, 2 equiv). Acetic acid was added to obtain a pH of 6-7 and the reaction was warmed at 60 °C for 18 h. An additional 2 equivalents of 4-bromobenzaldehyde and sodium cyanoborohydride were added after 18, 42 and 66 hours while maintaining the pH at 6-7 with acetic acid. After warming 90 h at 60°C, the reaction was concentrated and the residue was partitioned between EtOAc and aqueous saturated $NaHCO_3$ solution. The organic layer was washed with brine, dried ($MgSO_4$) and concentrated. The residue was purified by flash chromatography. Elution with EtOAc to 5 % NH_3-EtOH/EtOAC gave 3-benzyl-2-(1-{(4-bromobenzyl)[2-(dimethylamino)ethyl]amino}propyl)thieno[2,3-*d*]pyrimidin-4(3*H*)-one(8-1) as a pale yellow gum. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 (d, J = 6 Hz, 1H), 7.33 (d, J = 8 Hz, 2H), 7.21 (m, 4H), 7.05 (d, J = 8 Hz, 2H), 6.84 (d, J = 7 Hz, 2H), 5.85 (d, J = 16 Hz, 1H), 5.32 (d, J = 16 Hz, 1H), 3.87 (d, J = 14 Hz, 1H), 3.73 (dd, J = 11, 3 Hz, 1H), 3.50 (d, J = 14 Hz, 1H), 2.92 (m, 1H), 2.61 (m, 1H), 2.28 (m, 2H), 2.15 (m, 1H), 2.07 (s, 6H), 1.74 (m, 1H), 0.64 (t, J = 7 Hz, 3H).

TABLE 1

```
REMARK complex 1 with water molecules surrounding it
REMARK r= 0.2114 free_r= 0.2639
REMARK rmsd bonds= 0.006712  rmsd angles=  1.32262
REMARK B rmsd for bonded mainchain atoms=  1.570  target= 1.5
REMARK B rmsd for bonded sidechain atoms=  2.570  target= 2.0
REMARK B rmsd for angle mainchain atoms=  2.729  target= 2.0
REMARK B rmsd for angle sidechain atoms=  3.936  target= 2.5
REMARK sg= P2(1)2(1)2(1) a= 69.48 b= 79.54 c= 158.98 alpha= 90. beta= 90. gamma= 90.
REMARK reflection file= k2a.cv
REMARK B-correction resolution: 6.0 - 2.5
REMARK FILENAME="kin_16dpb.pdb"
ATOM      1  CB  ASN    18      37.472  -7.942 100.393  1.00 28.28      A
ATOM      2  CG  ASN    18      38.236  -7.260 101.506  1.00 31.25      A
ATOM      3  OD1 ASN    18      38.752  -7.913 102.413  1.00 36.19      A
ATOM      4  ND2 ASN    18      38.310  -5.940 101.448  1.00 32.46      A
ATOM      5  C   ASN    18      35.178  -7.311 101.124  1.00 24.09      A
ATOM      6  O   ASN    18      34.900  -6.997 102.284  1.00 23.76      A
ATOM      7  N   ASN    18      35.576  -9.454  99.859  1.00 25.44      A
ATOM      8  CA  ASN    18      36.124  -8.484 100.856  1.00 25.50      A
ATOM      9  N   ILE    19      34.708  -6.636 100.074  1.00 21.79      A
ATOM     10  CA  ILE    19      33.759  -5.540 100.278  1.00 19.48      A
ATOM     11  CB  ILE    19      33.425  -4.791  98.970  1.00 20.49      A
ATOM     12  CG2 ILE    19      32.124  -3.992  99.129  1.00 19.87      A
ATOM     13  CG1 ILE    19      34.573  -3.846  98.613  1.00 20.82      A
ATOM     14  CD1 ILE    19      34.194  -2.801  97.563  1.00 19.23      A
ATOM     15  C   ILE    19      32.487  -6.185 100.820  1.00 18.08      A
ATOM     16  O   ILE    19      31.929  -7.079 100.190  1.00 17.25      A
ATOM     17  N   GLN    20      32.044  -5.743 101.991  1.00 16.72      A
ATOM     18  CA  GLN    20      30.863  -6.315 102.624  1.00 17.94      A
ATOM     19  CB  GLN    20      30.996  -6.207 104.143  1.00 18.71      A
ATOM     20  CG  GLN    20      32.221  -6.950 104.689  1.00 19.97      A
ATOM     21  CD  GLN    20      32.369  -6.829 106.196  1.00 21.29      A
ATOM     22  OE1 GLN    20      32.511  -5.730 106.734  1.00 22.63      A
ATOM     23  NE2 GLN    20      32.336  -7.964 106.885  1.00 22.16      A
ATOM     24  C   GLN    20      29.560  -5.681 102.147  1.00 17.78      A
ATOM     25  O   GLN    20      29.396  -4.462 102.184  1.00 19.12      A
ATOM     26  N   VAL    21      28.640  -6.528 101.695  1.00 14.78      A
ATOM     27  CA  VAL    21      27.355  -6.080 101.176  1.00 13.75      A
ATOM     28  CB  VAL    21      27.144  -6.609  99.738  1.00 14.14      A
ATOM     29  CG1 VAL    21      25.854  -6.065  99.155  1.00 11.78      A
ATOM     30  CG2 VAL    21      28.339  -6.238  98.875  1.00 13.09      A
ATOM     31  C   VAL    21      26.198  -6.571 102.036  1.00 14.04      A
ATOM     32  O   VAL    21      26.128  -7.756 102.365  1.00 13.35      A
ATOM     33  N   VAL    22      25.294  -5.659 102.396  1.00 14.49      A
ATOM     34  CA  VAL    22      24.123  -6.011 103.194  1.00 14.01      A
ATOM     35  CB  VAL    22      24.197  -5.423 104.627  1.00 15.50      A
ATOM     36  CG1 VAL    22      25.588  -5.628 105.201  1.00 16.80      A
ATOM     37  CG2 VAL    22      23.817  -3.968 104.623  1.00 15.97      A
ATOM     38  C   VAL    22      22.838  -5.518 102.532  1.00 13.29      A
ATOM     39  O   VAL    22      22.811  -4.469 101.884  1.00 13.40      A
ATOM     40  N   VAL    23      21.773  -6.292 102.694  1.00 12.04      A
ATOM     41  CA  VAL    23      20.478  -5.953 102.125  1.00 11.16      A
ATOM     42  CB  VAL    23      19.890  -7.155 101.350  1.00 10.39      A
ATOM     43  CG1 VAL    23      18.423  -6.883 100.979  1.00  6.97      A
ATOM     44  CG2 VAL    23      20.733  -7.429 100.112  1.00  5.75      A
ATOM     45  C   VAL    23      19.496  -5.551 103.220  1.00 12.26      A
ATOM     46  O   VAL    23      19.433  -6.180 104.276  1.00 12.72      A
ATOM     47  N   ARG    24      18.734  -4.497 102.965  1.00 12.29      A
ATOM     48  CA  ARG    24      17.741  -4.033 103.925  1.00 11.98      A
ATOM     49  CB  ARG    24      18.150  -2.711 104.572  1.00  9.94      A
ATOM     50  CG  ARG    24      17.092  -2.197 105.533  1.00  9.40      A
ATOM     51  CD  ARG    24      17.412  -0.826 106.110  1.00 11.24      A
ATOM     52  NE  ARG    24      16.638  -0.585 107.326  1.00  8.87      A
ATOM     53  CZ  ARG    24      16.668   0.540 108.033  1.00 11.40      A
ATOM     54  NH1 ARG    24      17.432   1.563 107.649  1.00 11.52      A
ATOM     55  NH2 ARG    24      15.956   0.629 109.151  1.00 12.63      A
ATOM     56  C   ARG    24      16.404  -3.831 103.230  1.00 13.62      A
ATOM     57  O   ARG    24      16.248  -2.918 102.415  1.00 14.61      A
ATOM     58  N   CYS    25      15.446  -4.690 103.553  1.00 12.77      A
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ATOM	59	CA	CYS	25	14.117	-4.599	102.983	1.00	13.88	A
ATOM	60	CB	CYS	25	13.461	-5.980	102.951	1.00	15.60	A
ATOM	61	SG	CYS	25	11.855	-6.006	102.134	1.00	21.58	A
ATOM	62	C	CYS	25	13.292	-3.675	103.865	1.00	13.78	A
ATOM	63	O	CYS	25	13.293	-3.820	105.084	1.00	15.62	A
ATOM	64	N	ARG	26	12.605	-2.713	103.261	1.00	12.12	A
ATOM	65	CA	ARG	26	11.774	-1.815	104.045	1.00	12.61	A
ATOM	66	CB	ARG	26	11.601	-0.465	103.343	1.00	10.76	A
ATOM	67	CG	ARG	26	10.679	-0.499	102.128	1.00	7.66	A
ATOM	68	CD	ARG	26	10.181	0.890	101.775	1.00	7.16	A
ATOM	69	NE	ARG	26	9.592	0.934	100.442	1.00	7.55	A
ATOM	70	CZ	ARG	26	8.413	0.411	100.125	1.00	8.80	A
ATOM	71	NH1	ARG	26	7.677	-0.194	101.052	1.00	8.81	A
ATOM	72	NH2	ARG	26	7.980	0.472	98.876	1.00	7.02	A
ATOM	73	C	ARG	26	10.407	-2.470	104.215	1.00	15.65	A
ATOM	74	O	ARG	26	10.058	-3.420	103.500	1.00	17.10	A
ATOM	75	N	PRO	27	9.615	-1.982	105.170	1.00	17.31	A
ATOM	76	CD	PRO	27	9.957	-1.053	106.262	1.00	18.01	A
ATOM	77	CA	PRO	27	8.287	-2.562	105.382	1.00	20.54	A
ATOM	78	CB	PRO	27	8.037	-2.277	106.858	1.00	19.92	A
ATOM	79	CG	PRO	27	8.639	-0.932	107.017	1.00	17.88	A
ATOM	80	C	PRO	27	7.237	-1.897	104.492	1.00	23.41	A
ATOM	81	O	PRO	27	7.482	-0.833	103.916	1.00	23.28	A
ATOM	82	N	PHE	28	6.080	-2.542	104.371	1.00	26.52	A
ATOM	83	CA	PHE	28	4.976	-2.003	103.584	1.00	29.18	A
ATOM	84	CB	PHE	28	3.805	-2.982	103.588	1.00	27.65	A
ATOM	85	CG	PHE	28	3.948	-4.107	102.610	1.00	28.35	A
ATOM	86	CD1	PHE	28	3.947	-5.425	103.045	1.00	28.03	A
ATOM	87	CD2	PHE	28	4.038	-3.850	101.243	1.00	27.68	A
ATOM	88	CE1	PHE	28	4.026	-6.477	102.139	1.00	27.56	A
ATOM	89	CE2	PHE	28	4.119	-4.893	100.324	1.00	29.26	A
ATOM	90	CZ	PHE	28	4.112	-6.212	100.773	1.00	27.81	A
ATOM	91	C	PHE	28	4.513	-0.680	104.191	1.00	32.56	A
ATOM	92	O	PHE	28	4.426	-0.548	105.411	1.00	33.43	A
ATOM	93	N	ASN	29	4.217	0.299	103.345	1.00	37.21	A
ATOM	94	CA	ASN	29	3.744	1.595	103.829	1.00	42.32	A
ATOM	95	CB	ASN	29	4.073	2.692	102.809	1.00	42.04	A
ATOM	96	CG	ASN	29	3.604	2.344	101.410	1.00	41.31	A
ATOM	97	OD1	ASN	29	2.409	2.177	101.168	1.00	41.82	A
ATOM	98	ND2	ASN	29	4.546	2.228	100.482	1.00	40.11	A
ATOM	99	C	ASN	29	2.232	1.526	104.054	1.00	46.51	A
ATOM	100	O	ASN	29	1.606	0.505	103.768	1.00	46.59	A
ATOM	101	N	LEU	30	1.650	2.612	104.562	1.00	51.19	A
ATOM	102	CA	LEU	30	0.212	2.661	104.826	1.00	54.81	A
ATOM	103	CB	LEU	30	-0.178	4.040	105.362	1.00	56.40	A
ATOM	104	CG	LEU	30	-1.659	4.234	105.705	1.00	58.19	A
ATOM	105	CD1	LEU	30	-2.058	3.273	106.820	1.00	57.83	A
ATOM	106	CD2	LEU	30	-1.899	5.680	106.130	1.00	59.11	A
ATOM	107	C	LEU	30	-0.637	2.343	103.592	1.00	56.70	A
ATOM	108	O	LEU	30	-1.552	1.525	103.658	1.00	56.66	A
ATOM	109	N	ALA	31	-0.329	2.992	102.471	1.00	59.03	A
ATOM	110	CA	ALA	31	-1.062	2.787	101.222	1.00	61.19	A
ATOM	111	CB	ALA	31	-0.414	3.591	100.100	1.00	61.28	A
ATOM	112	C	ALA	31	-1.125	1.316	100.833	1.00	62.78	A
ATOM	113	O	ALA	31	-2.123	0.850	100.282	1.00	62.16	A
ATOM	114	N	GLU	32	-0.048	0.593	101.117	1.00	65.22	A
ATOM	115	CA	GLU	32	0.031	-0.827	100.801	1.00	67.27	A
ATOM	116	CB	GLU	32	1.501	-1.249	100.702	1.00	66.96	A
ATOM	117	CG	GLU	32	2.199	-0.712	99.453	1.00	67.12	A
ATOM	118	CD	GLU	32	3.713	-0.641	99.590	1.00	67.26	A
ATOM	119	OE1	GLU	32	4.392	-0.422	98.563	1.00	66.83	A
ATOM	120	OE2	GLU	32	4.223	-0.792	100.723	1.00	65.99	A
ATOM	121	C	GLU	32	-0.706	-1.666	101.844	1.00	68.26	A
ATOM	122	O	GLU	32	-1.260	-2.716	101.526	1.00	68.16	A
ATOM	123	N	ARG	33	-0.722	-1.191	103.087	1.00	69.65	A
ATOM	124	CA	ARG	33	-1.403	-1.897	104.169	1.00	71.22	A
ATOM	125	CB	ARG	33	-1.196	-1.162	105.498	1.00	72.33	A
ATOM	126	CG	ARG	33	0.239	-1.138	106.009	1.00	73.65	A
ATOM	127	CD	ARG	33	0.695	-2.508	106.479	1.00	74.57	A
ATOM	128	NE	ARG	33	2.043	-2.462	107.041	1.00	76.44	A
ATOM	129	CZ	ARG	33	2.692	-3.517	107.521	1.00	76.91	A
ATOM	130	NH1	ARG	33	2.119	-4.714	107.513	1.00	76.68	A
ATOM	131	NH2	ARG	33	3.918	-3.376	108.007	1.00	77.35	A

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ATOM    132  C   ARG    33      -2.901  -2.013 103.885  1.00 71.74      A
ATOM    133  O   ARG    33      -3.464  -3.111 103.900  1.00 71.46      A
ATOM    134  N   LYS    34      -3.536  -0.870 103.632  1.00 71.80      A
ATOM    135  CA  LYS    34      -4.967  -0.817 103.349  1.00 71.67      A
ATOM    136  CB  LYS    34      -5.426   0.641 103.195  1.00 72.94      A
ATOM    137  CG  LYS    34      -4.734   1.407 102.072  1.00 74.72      A
ATOM    138  CD  LYS    34      -5.218   2.856 101.986  1.00 75.69      A
ATOM    139  CE  LYS    34      -6.680   2.936 101.565  1.00 75.79      A
ATOM    140  NZ  LYS    34      -7.149   4.343 101.426  1.00 74.45      A
ATOM    141  C   LYS    34      -5.315  -1.604 102.088  1.00 70.68      A
ATOM    142  O   LYS    34      -6.448  -2.064 101.924  1.00 70.80      A
ATOM    143  N   ALA    35      -4.338  -1.753 101.198  1.00 68.59      A
ATOM    144  CA  ALA    35      -4.539  -2.501  99.963  1.00 66.37      A
ATOM    145  CB  ALA    35      -3.639  -1.949  98.861  1.00 65.65      A
ATOM    146  C   ALA    35      -4.199  -3.960 100.241  1.00 64.89      A
ATOM    147  O   ALA    35      -4.277  -4.807  99.352  1.00 64.01      A
ATOM    148  N   SER    36      -3.825  -4.233 101.491  1.00 63.72      A
ATOM    149  CA  SER    36      -3.454  -5.574 101.937  1.00 62.31      A
ATOM    150  CB  SER    36      -4.711  -6.422 102.194  1.00 62.73      A
ATOM    151  OG  SER    36      -5.556  -6.469 101.056  1.00 63.14      A
ATOM    152  C   SER    36      -2.542  -6.261 100.920  1.00 60.52      A
ATOM    153  O   SER    36      -2.933  -7.223 100.256  1.00 60.52      A
ATOM    154  N   ALA    37      -1.316  -5.759 100.818  1.00 57.81      A
ATOM    155  CA  ALA    37      -0.339  -6.291  99.877  1.00 54.58      A
ATOM    156  CB  ALA    37       0.709  -5.228  99.561  1.00 53.39      A
ATOM    157  C   ALA    37       0.351  -7.562 100.359  1.00 51.84      A
ATOM    158  O   ALA    37       0.586  -7.754 101.554  1.00 50.84      A
ATOM    159  N   HIS    38       0.669  -8.429  99.405  1.00 48.60      A
ATOM    160  CA  HIS    38       1.363  -9.672  99.690  1.00 45.12      A
ATOM    161  CB  HIS    38       0.775 -10.810  98.840  1.00 48.05      A
ATOM    162  CG  HIS    38       0.753 -10.528  97.364  1.00 50.18      A
ATOM    163  CD2 HIS    38      -0.262 -10.171  96.542  1.00 51.32      A
ATOM    164  ND1 HIS    38       1.875 -10.621  96.566  1.00 50.53      A
ATOM    165  CE1 HIS    38       1.552 -10.337  95.317  1.00 50.82      A
ATOM    166  NE2 HIS    38       0.261 -10.059  95.275  1.00 51.95      A
ATOM    167  C   HIS    38       2.836  -9.436  99.350  1.00 40.69      A
ATOM    168  O   HIS    38       3.165  -9.005  98.244  1.00 39.51      A
ATOM    169  N   SER    39       3.714  -9.692 100.312  1.00 34.50      A
ATOM    170  CA  SER    39       5.138  -9.494 100.106  1.00 29.81      A
ATOM    171  CB  SER    39       5.860  -9.458 101.449  1.00 29.59      A
ATOM    172  OG  SER    39       7.263  -9.361 101.265  1.00 30.93      A
ATOM    173  C   SER    39       5.753 -10.578  99.242  1.00 27.18      A
ATOM    174  O   SER    39       5.507 -11.758  99.456  1.00 27.84      A
ATOM    175  N   ILE    40       6.556 -10.179  98.263  1.00 23.70      A
ATOM    176  CA  ILE    40       7.216 -11.148  97.403  1.00 20.93      A
ATOM    177  CB  ILE    40       7.278 -10.677  95.945  1.00 21.59      A
ATOM    178  CG2 ILE    40       5.868 -10.554  95.381  1.00 21.07      A
ATOM    179  CG1 ILE    40       8.025  -9.343  95.857  1.00 21.01      A
ATOM    180  CD1 ILE    40       8.377  -8.954  94.443  1.00 17.86      A
ATOM    181  C   ILE    40       8.638 -11.366  97.895  1.00 19.29      A
ATOM    182  O   ILE    40       9.395 -12.130  97.306  1.00 18.82      A
ATOM    183  N   VAL    41       8.987 -10.696  98.988  1.00 18.43      A
ATOM    184  CA  VAL    41      10.316 -10.801  99.572  1.00 19.01      A
ATOM    185  CB  VAL    41      10.974  -9.394  99.666  1.00 18.10      A
ATOM    186  CG1 VAL    41      12.231  -9.448 100.525  1.00 17.03      A
ATOM    187  CG2 VAL    41      11.303  -8.881  98.279  1.00 16.81      A
ATOM    188  C   VAL    41      10.286 -11.420 100.976  1.00 21.10      A
ATOM    189  O   VAL    41       9.401 -11.122 101.779  1.00 22.16      A
ATOM    190  N   GLU    42      11.247 -12.286 101.269  1.00 21.96      A
ATOM    191  CA  GLU    42      11.336 -12.894 102.595  1.00 24.43      A
ATOM    192  CB  GLU    42      10.758 -14.310 102.588  1.00 26.41      A
ATOM    193  CG  GLU    42       9.235 -14.321 102.535  1.00 33.53      A
ATOM    194  CD  GLU    42       8.646 -15.717 102.435  1.00 37.53      A
ATOM    195  OE1 GLU    42       7.400 -15.830 102.388  1.00 37.91      A
ATOM    196  OE2 GLU    42       9.425 -16.695 102.399  1.00 39.48      A
ATOM    197  C   GLU    42      12.790 -12.912 103.042  1.00 23.06      A
ATOM    198  O   GLU    42      13.672 -13.313 102.284  1.00 23.11      A
ATOM    199  N   CYS    43      13.040 -12.461 104.267  1.00 22.56      A
ATOM    200  CA  CYS    43      14.399 -12.417 104.792  1.00 22.27      A
ATOM    201  CB  CYS    43      14.688 -11.032 105.350  1.00 21.27      A
ATOM    202  SG  CYS    43      14.515  -9.727 104.119  1.00 26.40      A
ATOM    203  C   CYS    43      14.683 -13.458 105.861  1.00 23.32      A
ATOM    204  O   CYS    43      13.795 -13.850 106.617  1.00 25.24      A
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ATOM	205	N	ASP	44	15.936	-13.900	105.909	1.00	24.35	A
ATOM	206	CA	ASP	44	16.398	-14.897	106.873	1.00	24.49	A
ATOM	207	CB	ASP	44	16.579	-16.251	106.182	1.00	24.72	A
ATOM	208	CG	ASP	44	16.638	-17.408	107.164	1.00	27.03	A
ATOM	209	OD1	ASP	44	17.089	-17.201	108.313	1.00	28.16	A
ATOM	210	OD2	ASP	44	16.249	-18.531	106.780	1.00	27.08	A
ATOM	211	C	ASP	44	17.745	-14.403	107.404	1.00	24.36	A
ATOM	212	O	ASP	44	18.804	-14.795	106.923	1.00	23.06	A
ATOM	213	N	PRO	45	17.721	-13.527	108.411	1.00	25.65	A
ATOM	214	CD	PRO	45	16.551	-12.911	109.059	1.00	25.98	A
ATOM	215	CA	PRO	45	18.967	-12.999	108.971	1.00	26.11	A
ATOM	216	CB	PRO	45	18.482	-12.143	110.133	1.00	25.67	A
ATOM	217	CG	PRO	45	17.153	-11.658	109.657	1.00	26.57	A
ATOM	218	C	PRO	45	19.972	-14.051	109.418	1.00	26.95	A
ATOM	219	O	PRO	45	21.159	-13.952	109.111	1.00	26.64	A
ATOM	220	N	VAL	46	19.502	-15.059	110.140	1.00	27.42	A
ATOM	221	CA	VAL	46	20.401	-16.088	110.636	1.00	28.91	A
ATOM	222	CB	VAL	46	19.634	-17.105	111.522	1.00	28.55	A
ATOM	223	CG1	VAL	46	18.882	-18.096	110.655	1.00	28.05	A
ATOM	224	CG2	VAL	46	20.600	-17.807	112.465	1.00	28.65	A
ATOM	225	C	VAL	46	21.148	-16.810	109.506	1.00	30.17	A
ATOM	226	O	VAL	46	22.279	-17.264	109.688	1.00	29.93	A
ATOM	227	N	ARG	47	20.530	-16.893	108.333	1.00	30.73	A
ATOM	228	CA	ARG	47	21.161	-17.552	107.195	1.00	31.90	A
ATOM	229	CB	ARG	47	20.156	-18.495	106.515	1.00	35.93	A
ATOM	230	CG	ARG	47	19.909	-19.796	107.286	1.00	43.15	A
ATOM	231	CD	ARG	47	18.670	-20.554	106.799	1.00	48.31	A
ATOM	232	NE	ARG	47	18.660	-20.769	105.352	1.00	52.94	A
ATOM	233	CZ	ARG	47	17.705	-21.426	104.697	1.00	53.97	A
ATOM	234	NH1	ARG	47	16.675	-21.940	105.356	1.00	54.33	A
ATOM	235	NH2	ARG	47	17.773	-21.561	103.381	1.00	54.58	A
ATOM	236	C	ARG	47	21.736	-16.560	106.171	1.00	30.25	A
ATOM	237	O	ARG	47	22.232	-16.965	105.122	1.00	27.99	A
ATOM	238	N	LYS	48	21.682	-15.266	106.484	1.00	29.50	A
ATOM	239	CA	LYS	48	22.200	-14.228	105.586	1.00	28.39	A
ATOM	240	CB	LYS	48	23.719	-14.362	105.425	1.00	28.24	A
ATOM	241	CG	LYS	48	24.497	-14.762	106.662	1.00	29.13	A
ATOM	242	CD	LYS	48	24.560	-13.656	107.677	1.00	31.53	A
ATOM	243	CE	LYS	48	25.701	-13.897	108.651	1.00	34.18	A
ATOM	244	NZ	LYS	48	27.015	-13.908	107.950	1.00	34.16	A
ATOM	245	C	LYS	48	21.564	-14.415	104.209	1.00	27.13	A
ATOM	246	O	LYS	48	22.244	-14.330	103.188	1.00	27.94	A
ATOM	247	N	GLU	49	20.261	-14.645	104.170	1.00	25.69	A
ATOM	248	CA	GLU	49	19.616	-14.908	102.895	1.00	26.19	A
ATOM	249	CB	GLU	49	19.300	-16.398	102.827	1.00	28.94	A
ATOM	250	CG	GLU	49	18.711	-16.897	101.534	1.00	34.48	A
ATOM	251	CD	GLU	49	18.082	-18.269	101.710	1.00	39.36	A
ATOM	252	OE1	GLU	49	16.880	-18.326	102.067	1.00	40.10	A
ATOM	253	OE2	GLU	49	18.794	-19.285	101.516	1.00	39.93	A
ATOM	254	C	GLU	49	18.355	-14.113	102.607	1.00	24.38	A
ATOM	255	O	GLU	49	17.545	-13.868	103.496	1.00	24.72	A
ATOM	256	N	VAL	50	18.196	-13.715	101.349	1.00	22.04	A
ATOM	257	CA	VAL	50	17.010	-12.989	100.928	1.00	21.18	A
ATOM	258	CB	VAL	50	17.350	-11.553	100.410	1.00	21.63	A
ATOM	259	CG1	VAL	50	18.150	-11.619	99.127	1.00	21.68	A
ATOM	260	CG2	VAL	50	16.071	-10.764	100.190	1.00	21.12	A
ATOM	261	C	VAL	50	16.392	-13.834	99.821	1.00	19.98	A
ATOM	262	O	VAL	50	17.088	-14.282	98.912	1.00	20.15	A
ATOM	263	N	SER	51	15.087	-14.074	99.917	1.00	21.09	A
ATOM	264	CA	SER	51	14.368	-14.890	98.934	1.00	21.32	A
ATOM	265	CB	SER	51	13.742	-16.106	99.629	1.00	20.35	A
ATOM	266	OG	SER	51	13.065	-16.943	98.712	1.00	23.49	A
ATOM	267	C	SER	51	13.280	-14.067	98.256	1.00	20.53	A
ATOM	268	O	SER	51	12.496	-13.401	98.925	1.00	21.64	A
ATOM	269	N	VAL	52	13.237	-14.107	96.929	1.00	21.28	A
ATOM	270	CA	VAL	52	12.238	-13.348	96.189	1.00	22.46	A
ATOM	271	CB	VAL	52	12.892	-12.293	95.282	1.00	21.66	A
ATOM	272	CG1	VAL	52	11.813	-11.462	94.605	1.00	18.69	A
ATOM	273	CG2	VAL	52	13.835	-11.417	96.091	1.00	19.80	A
ATOM	274	C	VAL	52	11.336	-14.220	95.322	1.00	24.82	A
ATOM	275	O	VAL	52	11.802	-15.099	94.597	1.00	26.25	A
ATOM	276	N	ARG	53	10.036	-13.964	95.409	1.00	27.28	A
ATOM	277	CA	ARG	53	9.034	-14.690	94.638	1.00	29.70	A

ATOM	278	CB	ARG	53	7.679	-14.562	95.341	1.00	29.44	A
ATOM	279	CG	ARG	53	6.511	-15.238	94.658	1.00	32.62	A
ATOM	280	CD	ARG	53	5.277	-15.124	95.536	1.00	32.33	A
ATOM	281	NE	ARG	53	5.486	-15.812	96.805	1.00	34.30	A
ATOM	282	CZ	ARG	53	4.754	-15.618	97.894	1.00	35.73	A
ATOM	283	NH1	ARG	53	3.751	-14.743	97.877	1.00	35.26	A
ATOM	284	NH2	ARG	53	5.029	-16.297	99.001	1.00	33.24	A
ATOM	285	C	ARG	53	8.992	-14.062	93.243	1.00	30.22	A
ATOM	286	O	ARG	53	8.554	-12.922	93.080	1.00	28.70	A
ATOM	287	N	THR	54	9.457	-14.809	92.244	1.00	32.13	A
ATOM	288	CA	THR	54	9.506	-14.314	90.872	1.00	35.09	A
ATOM	289	CB	THR	54	10.785	-14.788	90.153	1.00	34.03	A
ATOM	290	OG1	THR	54	10.798	-16.218	90.086	1.00	33.22	A
ATOM	291	CG2	THR	54	12.026	-14.305	90.898	1.00	33.36	A
ATOM	292	C	THR	54	8.317	-14.705	90.011	1.00	38.38	A
ATOM	293	O	THR	54	8.081	-14.098	88.970	1.00	39.08	A
ATOM	294	N	GLY	55	7.574	-15.717	90.435	1.00	42.35	A
ATOM	295	CA	GLY	55	6.433	-16.145	89.653	1.00	47.68	A
ATOM	296	C	GLY	55	5.137	-15.562	90.171	1.00	52.55	A
ATOM	297	O	GLY	55	4.638	-14.562	89.651	1.00	52.62	A
ATOM	298	N	GLY	56	4.589	-16.196	91.204	1.00	56.07	A
ATOM	299	CA	GLY	56	3.343	-15.734	91.789	1.00	58.64	A
ATOM	300	C	GLY	56	2.660	-16.804	92.620	1.00	60.65	A
ATOM	301	O	GLY	56	2.917	-17.999	92.444	1.00	60.57	A
ATOM	302	N	LEU	57	1.795	-16.364	93.532	1.00	62.43	A
ATOM	303	CA	LEU	57	1.039	-17.253	94.421	1.00	63.41	A
ATOM	304	CB	LEU	57	0.439	-18.425	93.627	1.00	63.91	A
ATOM	305	CG	LEU	57	-0.466	-18.152	92.419	1.00	64.67	A
ATOM	306	CD1	LEU	57	-0.951	-19.486	91.873	1.00	64.88	A
ATOM	307	CD2	LEU	57	-1.654	-17.276	92.806	1.00	64.92	A
ATOM	308	C	LEU	57	1.873	-17.800	95.586	1.00	63.25	A
ATOM	309	O	LEU	57	2.934	-18.393	95.383	1.00	63.31	A
ATOM	310	N	ALA	58	1.385	-17.591	96.807	1.00	62.63	A
ATOM	311	CA	ALA	58	2.063	-18.074	98.010	1.00	61.38	A
ATOM	312	CB	ALA	58	1.586	-17.286	99.229	1.00	60.84	A
ATOM	313	C	ALA	58	1.752	-19.562	98.184	1.00	60.68	A
ATOM	314	O	ALA	58	2.385	-20.261	98.979	1.00	60.38	A
ATOM	315	N	ASP	59	0.765	-20.024	97.422	1.00	59.38	A
ATOM	316	CA	ASP	59	0.321	-21.413	97.427	1.00	57.30	A
ATOM	317	CB	ASP	59	-1.058	-21.498	96.770	1.00	58.25	A
ATOM	318	CG	ASP	59	-1.438	-22.907	96.386	1.00	58.65	A
ATOM	319	OD1	ASP	59	-1.549	-23.767	97.285	1.00	58.25	A
ATOM	320	OD2	ASP	59	-1.628	-23.151	95.175	1.00	59.46	A
ATOM	321	C	ASP	59	1.314	-22.267	96.652	1.00	55.60	A
ATOM	322	O	ASP	59	1.588	-23.414	97.007	1.00	55.05	A
ATOM	323	N	LYS	60	1.849	-21.681	95.587	1.00	53.85	A
ATOM	324	CA	LYS	60	2.819	-22.340	94.718	1.00	51.83	A
ATOM	325	CB	LYS	60	2.099	-23.322	93.787	1.00	52.01	A
ATOM	326	CG	LYS	60	2.982	-23.940	92.720	1.00	51.22	A
ATOM	327	CD	LYS	60	2.184	-24.835	91.795	1.00	50.89	A
ATOM	328	CE	LYS	60	3.054	-25.341	90.663	1.00	52.06	A
ATOM	329	NZ	LYS	60	3.650	-24.213	89.891	1.00	52.67	A
ATOM	330	C	LYS	60	3.534	-21.258	93.900	1.00	50.64	A
ATOM	331	O	LYS	60	2.894	-20.350	93.358	1.00	51.26	A
ATOM	332	N	SER	61	4.855	-21.347	93.805	1.00	46.71	A
ATOM	333	CA	SER	61	5.582	-20.340	93.056	1.00	42.61	A
ATOM	334	CB	SER	61	5.478	-18.996	93.778	1.00	42.79	A
ATOM	335	OG	SER	61	6.132	-19.048	95.039	1.00	41.39	A
ATOM	336	C	SER	61	7.049	-20.668	92.846	1.00	40.50	A
ATOM	337	O	SER	61	7.581	-21.619	93.412	1.00	39.84	A
ATOM	338	N	SER	62	7.691	-19.856	92.017	1.00	37.70	A
ATOM	339	CA	SER	62	9.104	-19.998	91.732	1.00	34.42	A
ATOM	340	CB	SER	62	9.363	-19.776	90.245	1.00	34.68	A
ATOM	341	OG	SER	62	10.742	-19.881	89.964	1.00	38.74	A
ATOM	342	C	SER	62	9.796	-18.917	92.554	1.00	32.09	A
ATOM	343	O	SER	62	9.181	-17.903	92.888	1.00	29.47	A
ATOM	344	N	ARG	63	11.062	-19.126	92.896	1.00	30.00	A
ATOM	345	CA	ARG	63	11.775	-18.136	93.690	1.00	29.48	A
ATOM	346	CB	ARG	63	11.685	-18.472	95.189	1.00	31.57	A
ATOM	347	CG	ARG	63	10.273	-18.695	95.710	1.00	35.27	A
ATOM	348	CD	ARG	63	10.178	-18.504	97.218	1.00	37.21	A
ATOM	349	NE	ARG	63	10.260	-17.093	97.590	1.00	42.67	A
ATOM	350	CZ	ARG	63	9.885	-16.601	98.768	1.00	44.05	A

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ATOM    351  NH1 ARG    63       9.995 -15.299  99.014  1.00 42.72      A
ATOM    352  NH2 ARG    63       9.394 -17.408  99.700  1.00 46.01      A
ATOM    353  C   ARG    63      13.239 -17.994  93.314  1.00 27.46      A
ATOM    354  O   ARG    63      13.831 -18.887  92.702  1.00 26.59      A
ATOM    355  N   LYS    64      13.807 -16.853  93.693  1.00 25.59      A
ATOM    356  CA  LYS    64      15.216 -16.539  93.467  1.00 23.77      A
ATOM    357  CB  LYS    64      15.353 -15.299  92.587  1.00 25.43      A
ATOM    358  CG  LYS    64      15.991 -15.532  91.231  1.00 26.32      A
ATOM    359  CD  LYS    64      15.095 -16.338  90.323  1.00 28.26      A
ATOM    360  CE  LYS    64      15.692 -16.456  88.925  1.00 29.50      A
ATOM    361  NZ  LYS    64      15.825 -15.135  88.250  1.00 27.38      A
ATOM    362  C   LYS    64      15.808 -16.257  94.854  1.00 23.10      A
ATOM    363  O   LYS    64      15.244 -15.488  95.637  1.00 22.42      A
ATOM    364  N   THR    65      16.943 -16.876  95.154  1.00 22.03      A
ATOM    365  CA  THR    65      17.586 -16.715  96.452  1.00 20.67      A
ATOM    366  CB  THR    65      17.595 -18.081  97.179  1.00 21.12      A
ATOM    367  OG1 THR    65      16.352 -18.252  97.870  1.00 22.06      A
ATOM    368  CG2 THR    65      18.740 -18.187  98.154  1.00 27.20      A
ATOM    369  C   THR    65      19.002 -16.136  96.363  1.00 19.65      A
ATOM    370  O   THR    65      19.735 -16.430  95.425  1.00 22.34      A
ATOM    371  N   TYR    66      19.377 -15.300  97.331  1.00 17.01      A
ATOM    372  CA  TYR    66      20.714 -14.695  97.349  1.00 15.46      A
ATOM    373  CB  TYR    66      20.686 -13.244  96.829  1.00 14.31      A
ATOM    374  CG  TYR    66      20.034 -13.055  95.482  1.00 14.28      A
ATOM    375  CD1 TYR    66      18.651 -12.984  95.366  1.00 12.32      A
ATOM    376  CE1 TYR    66      18.046 -12.799  94.130  1.00 14.42      A
ATOM    377  CD2 TYR    66      20.804 -12.938  94.320  1.00 12.69      A
ATOM    378  CE2 TYR    66      20.207 -12.752  93.079  1.00 10.53      A
ATOM    379  CZ  TYR    66      18.829 -12.682  92.993  1.00 13.34      A
ATOM    380  OH  TYR    66      18.214 -12.483  91.776  1.00 14.95      A
ATOM    381  C   TYR    66      21.298 -14.675  98.754  1.00 14.50      A
ATOM    382  O   TYR    66      20.580 -14.461  99.733  1.00 13.73      A
ATOM    383  N   THR    67      22.605 -14.880  98.854  1.00 14.35      A
ATOM    384  CA  THR    67      23.260 -14.853 100.154  1.00 15.82      A
ATOM    385  CB  THR    67      24.083 -16.127 100.386  1.00 16.72      A
ATOM    386  OG1 THR    67      23.209 -17.261 100.418  1.00 17.16      A
ATOM    387  CG2 THR    67      24.845 -16.045 101.698  1.00 17.80      A
ATOM    388  C   THR    67      24.191 -13.650 100.203  1.00 16.72      A
ATOM    389  O   THR    67      24.992 -13.450  99.293  1.00 17.55      A
ATOM    390  N   PHE    68      24.071 -12.839 101.249  1.00 16.84      A
ATOM    391  CA  PHE    68      24.930 -11.666 101.405  1.00 18.85      A
ATOM    392  CB  PHE    68      24.119 -10.371 101.340  1.00 17.59      A
ATOM    393  CG  PHE    68      23.343 -10.206 100.080  1.00 17.32      A
ATOM    394  CD1 PHE    68      22.105 -10.823  99.926  1.00 16.89      A
ATOM    395  CD2 PHE    68      23.855  -9.447  99.036  1.00 17.68      A
ATOM    396  CE1 PHE    68      21.387 -10.680  98.752  1.00 15.86      A
ATOM    397  CE2 PHE    68      23.144  -9.296  97.852  1.00 16.89      A
ATOM    398  CZ  PHE    68      21.906  -9.916  97.708  1.00 17.47      A
ATOM    399  C   PHE    68      25.641 -11.731 102.745  1.00 19.38      A
ATOM    400  O   PHE    68      25.505 -12.703 103.479  1.00 21.74      A
ATOM    401  N   ASP    69      26.388 -10.688 103.078  1.00 19.56      A
ATOM    402  CA  ASP    69      27.105 -10.670 104.344  1.00 20.30      A
ATOM    403  CB  ASP    69      28.177  -9.571 104.313  1.00 20.07      A
ATOM    404  CG  ASP    69      29.306  -9.894 103.332  1.00 22.41      A
ATOM    405  OD1 ASP    69      29.245  -9.494 102.143  1.00 20.37      A
ATOM    406  OD2 ASP    69      30.259 -10.582 103.756  1.00 27.46      A
ATOM    407  C   ASP    69      26.150 -10.500 105.531  1.00 20.55      A
ATOM    408  O   ASP    69      26.369 -11.073 106.600  1.00 20.31      A
ATOM    409  N   MET    70      25.091  -9.718 105.325  1.00 21.04      A
ATOM    410  CA  MET    70      24.065  -9.469 106.338  1.00 20.59      A
ATOM    411  CB  MET    70      24.464  -8.322 107.257  1.00 23.87      A
ATOM    412  CG  MET    70      25.600  -8.650 108.202  1.00 27.55      A
ATOM    413  SD  MET    70      25.794  -7.359 109.420  1.00 28.63      A
ATOM    414  CE  MET    70      24.665  -7.914 110.676  1.00 29.22      A
ATOM    415  C   MET    70      22.737  -9.115 105.678  1.00 20.50      A
ATOM    416  O   MET    70      22.697  -8.426 104.657  1.00 19.82      A
ATOM    417  N   VAL    71      21.646  -9.593 106.258  1.00 18.11      A
ATOM    418  CA  VAL    71      20.335  -9.289 105.713  1.00 17.48      A
ATOM    419  CB  VAL    71      19.701 -10.516 105.021  1.00 17.16      A
ATOM    420  CG1 VAL    71      20.532 -10.915 103.802  1.00 14.56      A
ATOM    421  CG2 VAL    71      19.625 -11.662 105.986  1.00 19.68      A
ATOM    422  C   VAL    71      19.424  -8.791 106.822  1.00 16.09      A
ATOM    423  O   VAL    71      19.395  -9.350 107.913  1.00 14.72      A
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ATOM	424	N	PHE	72	18.714	-7.706	106.529	1.00	16.25		A
ATOM	425	CA	PHE	72	17.793	-7.075	107.460	1.00	15.53		A
ATOM	426	CB	PHE	72	18.289	-5.670	107.799	1.00	14.92		A
ATOM	427	CG	PHE	72	19.575	-5.658	108.575	1.00	17.03		A
ATOM	428	CD1	PHE	72	19.590	-6.004	109.925	1.00	16.20		A
ATOM	429	CD2	PHE	72	20.782	-5.332	107.950	1.00	17.34		A
ATOM	430	CE1	PHE	72	20.785	-6.026	110.649	1.00	16.42		A
ATOM	431	CE2	PHE	72	21.979	-5.352	108.660	1.00	16.87		A
ATOM	432	CZ	PHE	72	21.983	-5.702	110.016	1.00	16.79		A
ATOM	433	C	PHE	72	16.388	-7.007	106.874	1.00	15.43		A
ATOM	434	O	PHE	72	16.163	-6.394	105.834	1.00	13.98		A
ATOM	435	N	GLY	73	15.445	-7.646	107.557	1.00	18.08		A
ATOM	436	CA	GLY	73	14.067	-7.655	107.104	1.00	17.75		A
ATOM	437	C	GLY	73	13.343	-6.377	107.478	1.00	19.38		A
ATOM	438	O	GLY	73	13.918	-5.477	108.101	1.00	19.14		A
ATOM	439	N	ALA	74	12.069	-6.308	107.103	1.00	20.07		A
ATOM	440	CA	ALA	74	11.228	-5.145	107.363	1.00	20.00		A
ATOM	441	CB	ALA	74	9.840	-5.399	106.800	1.00	19.61		A
ATOM	442	C	ALA	74	11.124	-4.709	108.834	1.00	19.69		A
ATOM	443	O	ALA	74	10.972	-3.525	109.123	1.00	21.06		A
ATOM	444	N	SER	75	11.213	-5.650	109.765	1.00	18.30		A
ATOM	445	CA	SER	75	11.103	-5.300	111.177	1.00	18.31		A
ATOM	446	CB	SER	75	10.789	-6.553	111.991	1.00	16.40		A
ATOM	447	OG	SER	75	11.886	-7.450	111.971	1.00	15.90		A
ATOM	448	C	SER	75	12.359	-4.625	111.748	1.00	18.96		A
ATOM	449	O	SER	75	12.368	-4.196	112.902	1.00	19.99		A
ATOM	450	N	THR	76	13.407	-4.519	110.937	1.00	18.45		A
ATOM	451	CA	THR	76	14.667	-3.932	111.390	1.00	17.88		A
ATOM	452	CB	THR	76	15.783	-4.165	110.347	1.00	18.01		A
ATOM	453	OG1	THR	76	15.861	-5.567	110.019	1.00	17.20		A
ATOM	454	CG2	THR	76	17.109	-3.708	110.902	1.00	17.48		A
ATOM	455	C	THR	76	14.570	-2.437	111.687	1.00	17.40		A
ATOM	456	O	THR	76	14.064	-1.667	110.877	1.00	18.84		A
ATOM	457	N	LYS	77	15.061	-2.034	112.853	1.00	16.09		A
ATOM	458	CA	LYS	77	15.032	-0.633	113.262	1.00	17.09		A
ATOM	459	CB	LYS	77	14.667	-0.526	114.751	1.00	19.20		A
ATOM	460	CG	LYS	77	13.337	-1.181	115.120	1.00	20.20		A
ATOM	461	CD	LYS	77	12.198	-0.604	114.302	1.00	24.17		A
ATOM	462	CE	LYS	77	10.882	-1.325	114.556	1.00	28.56		A
ATOM	463	NZ	LYS	77	9.741	-0.673	113.832	1.00	29.29		A
ATOM	464	C	LYS	77	16.383	0.039	113.007	1.00	16.81		A
ATOM	465	O	LYS	77	17.382	-0.638	112.760	1.00	16.91		A
ATOM	466	N	GLN	78	16.414	1.368	113.067	1.00	14.39		A
ATOM	467	CA	GLN	78	17.657	2.101	112.831	1.00	13.21		A
ATOM	468	CB	GLN	78	17.422	3.611	112.945	1.00	10.26		A
ATOM	469	CG	GLN	78	16.343	4.179	112.017	1.00	10.24		A
ATOM	470	CD	GLN	78	16.799	4.325	110.579	1.00	8.85		A
ATOM	471	OE1	GLN	78	17.170	3.348	109.922	1.00	10.32		A
ATOM	472	NE2	GLN	78	16.776	5.555	110.081	1.00	6.58		A
ATOM	473	C	GLN	78	18.750	1.687	113.821	1.00	13.02		A
ATOM	474	O	GLN	78	19.933	1.636	113.474	1.00	11.38		A
ATOM	475	N	ILE	79	18.352	1.392	115.053	1.00	12.89		A
ATOM	476	CA	ILE	79	19.313	1.013	116.085	1.00	13.42		A
ATOM	477	CB	ILE	79	18.635	0.959	117.479	1.00	13.40		A
ATOM	478	CG2	ILE	79	17.591	-0.142	117.508	1.00	14.83		A
ATOM	479	CG1	ILE	79	19.684	0.733	118.571	1.00	13.65		A
ATOM	480	CD1	ILE	79	20.653	1.906	118.775	1.00	14.47		A
ATOM	481	C	ILE	79	19.972	-0.329	115.771	1.00	12.91		A
ATOM	482	O	ILE	79	21.157	-0.522	116.044	1.00	12.01		A
ATOM	483	N	ASP	80	19.204	-1.243	115.182	1.00	13.40		A
ATOM	484	CA	ASP	80	19.719	-2.555	114.815	1.00	14.93		A
ATOM	485	CB	ASP	80	18.581	-3.461	114.303	1.00	17.57		A
ATOM	486	CG	ASP	80	17.428	-3.593	115.300	1.00	20.41		A
ATOM	487	OD1	ASP	80	17.692	-3.811	116.504	1.00	22.08		A
ATOM	488	OD2	ASP	80	16.253	-3.492	114.879	1.00	21.37		A
ATOM	489	C	ASP	80	20.777	-2.393	113.719	1.00	15.46		A
ATOM	490	O	ASP	80	21.845	-3.007	113.769	1.00	15.07		A
ATOM	491	N	VAL	81	20.467	-1.560	112.730	1.00	15.97		A
ATOM	492	CA	VAL	81	21.380	-1.307	111.625	1.00	16.25		A
ATOM	493	CB	VAL	81	20.747	-0.360	110.555	1.00	16.07		A
ATOM	494	CG1	VAL	81	21.787	0.027	109.526	1.00	14.56		A
ATOM	495	CG2	VAL	81	19.568	-1.049	109.857	1.00	14.48		A
ATOM	496	C	VAL	81	22.667	-0.681	112.142	1.00	18.57		A

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ATOM    497  O   VAL   81      23.758  -1.079 111.733  1.00 20.96      A
ATOM    498  N   TYR   82      22.549   0.289 113.046  1.00 19.05      A
ATOM    499  CA  TYR   82      23.732   0.946 113.583  1.00 20.41      A
ATOM    500  CB  TYR   82      23.339   2.132 114.471  1.00 23.17      A
ATOM    501  CG  TYR   82      24.532   2.903 114.992  1.00 24.73      A
ATOM    502  CD1 TYR   82      25.137   2.556 116.198  1.00 24.58      A
ATOM    503  CE1 TYR   82      26.284   3.200 116.638  1.00 25.15      A
ATOM    504  CD2 TYR   82      25.107   3.928 114.237  1.00 25.38      A
ATOM    505  CE2 TYR   82      26.258   4.576 114.668  1.00 25.61      A
ATOM    506  CZ  TYR   82      26.842   4.204 115.868  1.00 25.89      A
ATOM    507  OH  TYR   82      28.000   4.818 116.297  1.00 26.74      A
ATOM    508  C   TYR   82      24.633  -0.002 114.375  1.00 22.16      A
ATOM    509  O   TYR   82      25.835  -0.104 114.103  1.00 22.17      A
ATOM    510  N   ARG   83      24.059  -0.694 115.352  1.00 21.11      A
ATOM    511  CA  ARG   83      24.834  -1.615 116.170  1.00 20.40      A
ATOM    512  CB  ARG   83      23.928  -2.263 117.222  1.00 18.85      A
ATOM    513  CG  ARG   83      23.521  -1.315 118.339  1.00 21.14      A
ATOM    514  CD  ARG   83      22.272  -1.804 119.065  1.00 21.88      A
ATOM    515  NE  ARG   83      22.478  -3.061 119.779  1.00 22.27      A
ATOM    516  CZ  ARG   83      23.184  -3.175 120.899  1.00 23.18      A
ATOM    517  NH1 ARG   83      23.757  -2.104 121.434  1.00 23.11      A
ATOM    518  NH2 ARG   83      23.308  -4.356 121.490  1.00 23.57      A
ATOM    519  C   ARG   83      25.553  -2.694 115.361  1.00 19.49      A
ATOM    520  O   ARG   83      26.702  -3.022 115.647  1.00 17.49      A
ATOM    521  N   SER   84      24.885  -3.225 114.341  1.00 19.74      A
ATOM    522  CA  SER   84      25.462  -4.283 113.519  1.00 19.67      A
ATOM    523  CB  SER   84      24.359  -5.135 112.888  1.00 21.49      A
ATOM    524  OG  SER   84      23.716  -5.931 113.865  1.00 28.64      A
ATOM    525  C   SER   84      26.419  -3.859 112.426  1.00 18.56      A
ATOM    526  O   SER   84      27.487  -4.436 112.302  1.00 19.77      A
ATOM    527  N   VAL   85      26.058  -2.866 111.624  1.00 18.63      A
ATOM    528  CA  VAL   85      26.949  -2.470 110.542  1.00 19.52      A
ATOM    529  CB  VAL   85      26.161  -2.241 109.222  1.00 19.26      A
ATOM    530  CG1 VAL   85      25.165  -3.377 109.011  1.00 20.45      A
ATOM    531  CG2 VAL   85      25.448  -0.925 109.251  1.00 22.19      A
ATOM    532  C   VAL   85      27.828  -1.252 110.810  1.00 19.41      A
ATOM    533  O   VAL   85      29.034  -1.289 110.558  1.00 19.81      A
ATOM    534  N   VAL   86      27.236  -0.189 111.342  1.00 19.42      A
ATOM    535  CA  VAL   86      27.959   1.053 111.603  1.00 19.60      A
ATOM    536  CB  VAL   86      26.971   2.226 111.815  1.00 18.59      A
ATOM    537  CG1 VAL   86      27.724   3.545 111.800  1.00 19.00      A
ATOM    538  CG2 VAL   86      25.899   2.208 110.736  1.00 18.56      A
ATOM    539  C   VAL   86      28.950   1.067 112.773  1.00 20.31      A
ATOM    540  O   VAL   86      30.060   1.584 112.637  1.00 19.36      A
ATOM    541  N   CYS   87      28.559   0.519 113.919  1.00 21.30      A
ATOM    542  CA  CYS   87      29.438   0.535 115.082  1.00 23.03      A
ATOM    543  CB  CYS   87      28.777  -0.187 116.254  1.00 26.09      A
ATOM    544  SG  CYS   87      29.481   0.238 117.859  1.00 36.72      A
ATOM    545  C   CYS   87      30.824  -0.056 114.804  1.00 21.77      A
ATOM    546  O   CYS   87      31.835   0.546 115.145  1.00 21.30      A
ATOM    547  N   PRO   88      30.894  -1.241 114.185  1.00 20.49      A
ATOM    548  CD  PRO   88      29.856  -2.240 113.881  1.00 20.97      A
ATOM    549  CA  PRO   88      32.231  -1.783 113.926  1.00 20.97      A
ATOM    550  CB  PRO   88      31.948  -3.215 113.473  1.00 18.41      A
ATOM    551  CG  PRO   88      30.571  -3.133 112.895  1.00 20.02      A
ATOM    552  C   PRO   88      33.052  -0.988 112.905  1.00 21.87      A
ATOM    553  O   PRO   88      34.280  -0.937 113.000  1.00 22.69      A
ATOM    554  N   ILE   89      32.380  -0.373 111.934  1.00 21.27      A
ATOM    555  CA  ILE   89      33.068   0.417 110.915  1.00 20.39      A
ATOM    556  CB  ILE   89      32.130   0.723 109.720  1.00 20.42      A
ATOM    557  CG2 ILE   89      32.791   1.710 108.762  1.00 16.94      A
ATOM    558  CG1 ILE   89      31.786  -0.584 108.998  1.00 20.17      A
ATOM    559  CD1 ILE   89      30.749  -0.429 107.886  1.00 21.44      A
ATOM    560  C   ILE   89      33.577   1.724 111.515  1.00 21.10      A
ATOM    561  O   ILE   89      34.640   2.214 111.144  1.00 22.45      A
ATOM    562  N   LEU   90      32.818   2.287 112.449  1.00 20.96      A
ATOM    563  CA  LEU   90      33.229   3.522 113.103  1.00 20.72      A
ATOM    564  CB  LEU   90      32.086   4.094 113.940  1.00 18.19      A
ATOM    565  CG  LEU   90      32.407   5.390 114.687  1.00 19.36      A
ATOM    566  CD1 LEU   90      32.779   6.495 113.702  1.00 17.91      A
ATOM    567  CD2 LEU   90      31.203   5.799 115.515  1.00 19.74      A
ATOM    568  C   LEU   90      34.443   3.248 113.989  1.00 21.43      A
ATOM    569  O   LEU   90      35.346   4.081 114.089  1.00 22.10      A
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ATOM	570	N	ASP	91	34.471	2.084	114.632	1.00	21.61	A
ATOM	571	CA	ASP	91	35.611	1.731	115.476	1.00	22.75	A
ATOM	572	CB	ASP	91	35.404	0.380	116.172	1.00	22.67	A
ATOM	573	CG	ASP	91	34.535	0.486	117.410	1.00	25.39	A
ATOM	574	OD1	ASP	91	34.386	1.604	117.947	1.00	24.95	A
ATOM	575	OD2	ASP	91	34.006	-0.552	117.859	1.00	27.30	A
ATOM	576	C	ASP	91	36.877	1.667	114.618	1.00	22.42	A
ATOM	577	O	ASP	91	37.956	2.039	115.077	1.00	20.39	A
ATOM	578	N	GLU	92	36.749	1.199	113.378	1.00	20.58	A
ATOM	579	CA	GLU	92	37.907	1.130	112.499	1.00	22.88	A
ATOM	580	CB	GLU	92	37.599	0.311	111.238	1.00	24.90	A
ATOM	581	CG	GLU	92	38.131	-1.120	111.282	1.00	31.75	A
ATOM	582	CD	GLU	92	38.517	-1.655	109.902	1.00	35.40	A
ATOM	583	OE1	GLU	92	39.330	-1.007	109.203	1.00	36.87	A
ATOM	584	OE2	GLU	92	38.017	-2.732	109.519	1.00	37.95	A
ATOM	585	C	GLU	92	38.358	2.537	112.100	1.00	22.24	A
ATOM	586	O	GLU	92	39.554	2.799	111.964	1.00	21.80	A
ATOM	587	N	VAL	93	37.398	3.438	111.909	1.00	20.21	A
ATOM	588	CA	VAL	93	37.712	4.808	111.532	1.00	18.97	A
ATOM	589	CB	VAL	93	36.422	5.626	111.228	1.00	17.93	A
ATOM	590	CG1	VAL	93	36.755	7.102	111.094	1.00	14.46	A
ATOM	591	CG2	VAL	93	35.781	5.124	109.937	1.00	16.29	A
ATOM	592	C	VAL	93	38.489	5.482	112.657	1.00	19.09	A
ATOM	593	O	VAL	93	39.477	6.174	112.414	1.00	18.02	A
ATOM	594	N	ILE	94	38.044	5.263	113.889	1.00	19.70	A
ATOM	595	CA	ILE	94	38.690	5.845	115.056	1.00	21.90	A
ATOM	596	CB	ILE	94	37.815	5.615	116.317	1.00	22.69	A
ATOM	597	CG2	ILE	94	38.519	6.128	117.571	1.00	22.60	A
ATOM	598	CG1	ILE	94	36.472	6.336	116.124	1.00	22.49	A
ATOM	599	CD1	ILE	94	35.480	6.155	117.266	1.00	22.50	A
ATOM	600	C	ILE	94	40.116	5.302	115.265	1.00	24.26	A
ATOM	601	O	ILE	94	40.924	5.931	115.945	1.00	24.34	A
ATOM	602	N	MET	95	40.428	4.148	114.672	1.00	25.73	A
ATOM	603	CA	MET	95	41.767	3.559	114.777	1.00	27.17	A
ATOM	604	CB	MET	95	41.732	2.047	114.532	1.00	29.33	A
ATOM	605	CG	MET	95	41.102	1.237	115.643	1.00	35.68	A
ATOM	606	SD	MET	95	41.281	-0.526	115.337	1.00	44.01	A
ATOM	607	CE	MET	95	39.718	-0.911	114.541	1.00	39.10	A
ATOM	608	C	MET	95	42.722	4.183	113.761	1.00	27.37	A
ATOM	609	O	MET	95	43.907	3.832	113.711	1.00	26.10	A
ATOM	610	N	GLY	96	42.197	5.088	112.939	1.00	26.75	A
ATOM	611	CA	GLY	96	43.020	5.753	111.941	1.00	26.52	A
ATOM	612	C	GLY	96	42.861	5.220	110.529	1.00	25.69	A
ATOM	613	O	GLY	96	43.752	5.373	109.690	1.00	25.52	A
ATOM	614	N	TYR	97	41.720	4.597	110.264	1.00	25.64	A
ATOM	615	CA	TYR	97	41.439	4.033	108.949	1.00	24.96	A
ATOM	616	CB	TYR	97	40.932	2.592	109.113	1.00	29.74	A
ATOM	617	CG	TYR	97	42.007	1.569	109.444	1.00	34.33	A
ATOM	618	CD1	TYR	97	42.993	1.243	108.514	1.00	36.66	A
ATOM	619	CE1	TYR	97	43.970	0.292	108.798	1.00	39.73	A
ATOM	620	CD2	TYR	97	42.025	0.914	110.680	1.00	35.77	A
ATOM	621	CE2	TYR	97	42.998	-0.037	110.979	1.00	38.01	A
ATOM	622	CZ	TYR	97	43.969	-0.342	110.033	1.00	40.42	A
ATOM	623	OH	TYR	97	44.956	-1.264	110.325	1.00	41.65	A
ATOM	624	C	TYR	97	40.407	4.854	108.163	1.00	22.65	A
ATOM	625	O	TYR	97	39.749	5.741	108.711	1.00	22.45	A
ATOM	626	N	ASN	98	40.290	4.565	106.872	1.00	19.89	A
ATOM	627	CA	ASN	98	39.312	5.226	106.021	1.00	18.57	A
ATOM	628	CB	ASN	98	39.941	5.682	104.702	1.00	19.70	A
ATOM	629	CG	ASN	98	40.867	6.863	104.873	1.00	21.50	A
ATOM	630	OD1	ASN	98	40.543	7.826	105.574	1.00	23.29	A
ATOM	631	ND2	ASN	98	42.020	6.807	104.222	1.00	20.02	A
ATOM	632	C	ASN	98	38.195	4.230	105.713	1.00	18.68	A
ATOM	633	O	ASN	98	38.459	3.087	105.346	1.00	16.93	A
ATOM	634	N	CYS	99	36.949	4.657	105.865	1.00	18.23	A
ATOM	635	CA	CYS	99	35.825	3.776	105.575	1.00	17.76	A
ATOM	636	CB	CYS	99	35.244	3.186	106.867	1.00	18.42	A
ATOM	637	SG	CYS	99	36.378	2.095	107.771	1.00	19.49	A
ATOM	638	C	CYS	99	34.727	4.481	104.790	1.00	15.84	A
ATOM	639	O	CYS	99	34.508	5.685	104.920	1.00	13.06	A
ATOM	640	N	THR	100	34.044	3.696	103.968	1.00	15.18	A
ATOM	641	CA	THR	100	32.968	4.190	103.130	1.00	14.06	A
ATOM	642	CB	THR	100	33.417	4.278	101.657	1.00	12.78	A

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ATOM    643  OG1 THR   100      34.485   5.223 101.539  1.00 14.13      A
ATOM    644  CG2 THR   100      32.262   4.717 100.773  1.00 12.44      A
ATOM    645  C   THR   100      31.759   3.260 103.200  1.00 14.15      A
ATOM    646  O   THR   100      31.907   2.034 103.263  1.00 13.80      A
ATOM    647  N   ILE   101      30.568   3.851 103.199  1.00 12.37      A
ATOM    648  CA  ILE   101      29.329   3.088 103.202  1.00 11.07      A
ATOM    649  CB  ILE   101      28.608   3.158 104.551  1.00 10.99      A
ATOM    650  CG2 ILE   101      27.404   2.213 104.527  1.00 11.07      A
ATOM    651  CG1 ILE   101      29.551   2.756 105.682  1.00 11.36      A
ATOM    652  CD1 ILE   101      28.880   2.767 107.071  1.00 11.31      A
ATOM    653  C   ILE   101      28.394   3.659 102.123  1.00 10.34      A
ATOM    654  O   ILE   101      28.077   4.842 102.133  1.00  8.62      A
ATOM    655  N   PHE   102      27.980   2.807 101.192  1.00  8.88      A
ATOM    656  CA  PHE   102      27.089   3.200 100.113  1.00  8.18      A
ATOM    657  CB  PHE   102      27.521   2.554  98.798  1.00  8.39      A
ATOM    658  CG  PHE   102      28.786   3.107  98.212  1.00  8.44      A
ATOM    659  CD1 PHE   102      28.746   4.237  97.400  1.00  8.21      A
ATOM    660  CD2 PHE   102      30.004   2.449  98.402  1.00  7.42      A
ATOM    661  CE1 PHE   102      29.901   4.712  96.770  1.00 10.64      A
ATOM    662  CE2 PHE   102      31.167   2.910  97.780  1.00  9.88      A
ATOM    663  CZ  PHE   102      31.119   4.044  96.957  1.00 10.26      A
ATOM    664  C   PHE   102      25.686   2.695 100.418  1.00  9.34      A
ATOM    665  O   PHE   102      25.514   1.676 101.084  1.00  9.83      A
ATOM    666  N   ALA   103      24.686   3.420  99.937  1.00  8.83      A
ATOM    667  CA  ALA   103      23.301   3.008 100.088  1.00  6.41      A
ATOM    668  CB  ALA   103      22.503   4.057 100.836  1.00  6.59      A
ATOM    669  C   ALA   103      22.887   2.920  98.619  1.00  5.06      A
ATOM    670  O   ALA   103      22.988   3.898  97.890  1.00  3.08      A
ATOM    671  N   TYR   104      22.476   1.735  98.184  1.00  4.26      A
ATOM    672  CA  TYR   104      22.110   1.498  96.791  1.00  4.91      A
ATOM    673  CB  TYR   104      23.142   0.552  96.137  1.00  3.89      A
ATOM    674  CG  TYR   104      22.911   0.238  94.666  1.00  4.19      A
ATOM    675  CD1 TYR   104      21.933  -0.675  94.260  1.00  6.04      A
ATOM    676  CE1 TYR   104      21.722  -0.946  92.898  1.00  7.93      A
ATOM    677  CD2 TYR   104      23.667   0.868  93.679  1.00  5.77      A
ATOM    678  CE2 TYR   104      23.466   0.608  92.326  1.00  5.74      A
ATOM    679  CZ  TYR   104      22.500  -0.295  91.944  1.00  6.93      A
ATOM    680  OH  TYR   104      22.326  -0.551  90.604  1.00  8.61      A
ATOM    681  C   TYR   104      20.718   0.893  96.678  1.00  5.23      A
ATOM    682  O   TYR   104      20.346   0.007  97.445  1.00  7.02      A
ATOM    683  N   GLY   105      19.955   1.368  95.704  1.00  3.82      A
ATOM    684  CA  GLY   105      18.620   0.857  95.521  1.00  5.02      A
ATOM    685  C   GLY   105      17.705   1.803  94.773  1.00  5.87      A
ATOM    686  O   GLY   105      17.981   2.992  94.590  1.00  6.06      A
ATOM    687  N   GLN   106      16.598   1.244  94.326  1.00  4.13      A
ATOM    688  CA  GLN   106      15.601   1.986  93.591  1.00  6.44      A
ATOM    689  CB  GLN   106      14.513   0.998  93.158  1.00  6.41      A
ATOM    690  CG  GLN   106      13.175   1.585  92.817  1.00 11.96      A
ATOM    691  CD  GLN   106      12.136   0.511  92.499  1.00 14.57      A
ATOM    692  OE1 GLN   106      12.060  -0.539  93.172  1.00 12.16      A
ATOM    693  NE2 GLN   106      11.318   0.774  91.483  1.00 10.80      A
ATOM    694  C   GLN   106      15.047   3.091  94.488  1.00  7.89      A
ATOM    695  O   GLN   106      15.083   2.992  95.725  1.00  8.30      A
ATOM    696  N   THR   107      14.558   4.157  93.869  1.00  8.49      A
ATOM    697  CA  THR   107      13.981   5.259  94.620  1.00  8.83      A
ATOM    698  CB  THR   107      13.532   6.371  93.668  1.00 10.17      A
ATOM    699  OG1 THR   107      14.681   6.936  93.023  1.00 11.92      A
ATOM    700  CG2 THR   107      12.783   7.464  94.431  1.00  9.05      A
ATOM    701  C   THR   107      12.763   4.751  95.392  1.00 11.60      A
ATOM    702  O   THR   107      11.936   4.017  94.838  1.00 13.74      A
ATOM    703  N   GLY   108      12.661   5.121  96.668  1.00 11.74      A
ATOM    704  CA  GLY   108      11.527   4.703  97.476  1.00  9.99      A
ATOM    705  C   GLY   108      11.738   3.461  98.330  1.00 11.25      A
ATOM    706  O   GLY   108      10.812   3.004  99.018  1.00 12.52      A
ATOM    707  N   THR   109      12.947   2.915  98.313  1.00  9.04      A
ATOM    708  CA  THR   109      13.216   1.716  99.090  1.00  8.13      A
ATOM    709  CB  THR   109      14.053   0.703  98.291  1.00  8.11      A
ATOM    710  OG1 THR   109      15.274   1.321  97.857  1.00  5.32      A
ATOM    711  CG2 THR   109      13.269   0.220  97.079  1.00  2.18      A
ATOM    712  C   THR   109      13.914   1.990 100.405  1.00  8.77      A
ATOM    713  O   THR   109      14.029   1.085 101.236  1.00  9.56      A
ATOM    714  N   GLY   110      14.411   3.211 100.599  1.00  6.93      A
ATOM    715  CA  GLY   110      15.037   3.517 101.878  1.00  7.00      A
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ATOM	716	C	GLY	110	16.491	3.959	101.985	1.00	8.39	A	
ATOM	717	O	GLY	110	17.052	3.953	103.089	1.00	6.64	A	
ATOM	718	N	LYS	111	17.106	4.346	100.869	1.00	8.77	A	
ATOM	719	CA	LYS	111	18.493	4.798	100.888	1.00	8.41	A	
ATOM	720	CB	LYS	111	18.938	5.257	99.495	1.00	9.46	A	
ATOM	721	CG	LYS	111	19.086	4.134	98.462	1.00	8.41	A	
ATOM	722	CD	LYS	111	19.650	4.651	97.133	1.00	7.10	A	
ATOM	723	CE	LYS	111	18.772	5.741	96.526	1.00	8.55	A	
ATOM	724	NZ	LYS	111	17.364	5.298	96.325	1.00	7.14	A	
ATOM	725	C	LYS	111	18.643	5.956	101.862	1.00	8.34	A	
ATOM	726	O	LYS	111	19.448	5.895	102.789	1.00	9.08	A	
ATOM	727	N	THR	112	17.851	7.006	101.651	1.00	8.83	A	
ATOM	728	CA	THR	112	17.896	8.198	102.502	1.00	7.73	A	
ATOM	729	CB	THR	112	17.027	9.342	101.903	1.00	8.07	A	
ATOM	730	OG1	THR	112	17.347	9.520	100.502	1.00	8.01	A	
ATOM	731	CG2	THR	112	17.287	10.650	102.650	1.00	4.02	A	
ATOM	732	C	THR	112	17.454	7.905	103.945	1.00	8.81	A	
ATOM	733	O	THR	112	17.997	8.458	104.894	1.00	8.08	A	
ATOM	734	N	PHE	113	16.476	7.025	104.114	1.00	11.03	A	
ATOM	735	CA	PHE	113	16.008	6.664	105.448	1.00	11.19	A	
ATOM	736	CB	PHE	113	14.806	5.727	105.361	1.00	10.34	A	
ATOM	737	CG	PHE	113	14.208	5.385	106.699	1.00	10.76	A	
ATOM	738	CD1	PHE	113	13.247	6.214	107.276	1.00	9.64	A	
ATOM	739	CD2	PHE	113	14.623	4.249	107.393	1.00	9.33	A	
ATOM	740	CE1	PHE	113	12.703	5.917	108.523	1.00	10.99	A	
ATOM	741	CE2	PHE	113	14.084	3.942	108.646	1.00	11.97	A	
ATOM	742	CZ	PHE	113	13.120	4.781	109.212	1.00	9.40	A	
ATOM	743	C	PHE	113	17.120	5.943	106.205	1.00	11.21	A	
ATOM	744	O	PHE	113	17.254	6.081	107.418	1.00	11.83	A	
ATOM	745	N	THR	114	17.908	5.159	105.483	1.00	10.89	A	
ATOM	746	CA	THR	114	18.992	4.422	106.101	1.00	9.91	A	
ATOM	747	CB	THR	114	19.458	3.267	105.173	1.00	12.09	A	
ATOM	748	OG1	THR	114	18.375	2.336	105.001	1.00	10.83	A	
ATOM	749	CG2	THR	114	20.677	2.537	105.763	1.00	9.73	A	
ATOM	750	C	THR	114	20.167	5.329	106.438	1.00	10.11	A	
ATOM	751	O	THR	114	20.650	5.328	107.569	1.00	10.60	A	
ATOM	752	N	MET	115	20.606	6.125	105.466	1.00	11.39	A	
ATOM	753	CA	MET	115	21.745	7.021	105.666	1.00	11.76	A	
ATOM	754	CB	MET	115	22.286	7.503	104.323	1.00	14.08	A	
ATOM	755	CG	MET	115	22.774	6.402	103.406	1.00	21.28	A	
ATOM	756	SD	MET	115	24.093	5.411	104.142	1.00	28.02	A	
ATOM	757	CE	MET	115	25.184	6.682	104.670	1.00	16.59	A	
ATOM	758	C	MET	115	21.489	8.240	106.547	1.00	11.39	A	
ATOM	759	O	MET	115	22.347	8.607	107.349	1.00	11.70	A	
ATOM	760	N	GLU	116	20.322	8.868	106.410	1.00	10.32	A	
ATOM	761	CA	GLU	116	20.023	10.064	107.197	1.00	9.04	A	
ATOM	762	CB	GLU	116	19.498	11.185	106.299	1.00	11.83	A	
ATOM	763	CG	GLU	116	20.215	11.349	104.970	1.00	15.21	A	
ATOM	764	CD	GLU	116	19.911	12.682	104.319	1.00	17.70	A	
ATOM	765	OE1	GLU	116	18.751	13.137	104.405	1.00	20.63	A	
ATOM	766	OE2	GLU	116	20.830	13.272	103.715	1.00	19.36	A	
ATOM	767	C	GLU	116	19.021	9.867	108.319	1.00	8.57	A	
ATOM	768	O	GLU	116	19.225	10.344	109.430	1.00	6.66	A	
ATOM	769	N	GLY	117	17.937	9.162	108.024	1.00	10.69	A	
ATOM	770	CA	GLY	117	16.894	8.961	109.011	1.00	12.05	A	
ATOM	771	C	GLY	117	15.906	10.119	108.921	1.00	14.49	A	
ATOM	772	O	GLY	117	16.009	10.967	108.030	1.00	15.09	A	
ATOM	773	N	GLU	118	14.954	10.176	109.844	1.00	15.27	A	
ATOM	774	CA	GLU	118	13.955	11.240	109.827	1.00	17.05	A	
ATOM	775	CB	GLU	118	12.680	10.764	109.132	1.00	18.95	A	
ATOM	776	CG	GLU	118	12.881	10.219	107.732	1.00	24.85	A	
ATOM	777	CD	GLU	118	11.659	9.462	107.228	1.00	28.50	A	
ATOM	778	OE1	GLU	118	11.639	9.064	106.047	1.00	29.02	A	
ATOM	779	OE2	GLU	118	10.715	9.260	108.025	1.00	31.54	A	
ATOM	780	C	GLU	118	13.601	11.631	111.246	1.00	15.85	A	
ATOM	781	O	GLU	118	14.159	11.111	112.206	1.00	17.29	A	
ATOM	782	N	ARG	119	12.660	12.549	111.381	1.00	14.03	A	
ATOM	783	CA	ARG	119	12.238	12.955	112.701	1.00	12.36	A	
ATOM	784	CB	ARG	119	12.058	14.469	112.765	1.00	9.51	A	
ATOM	785	CG	ARG	119	13.311	15.275	112.459	1.00	9.85	A	
ATOM	786	CD	ARG	119	14.517	14.768	113.223	1.00	9.11	A	
ATOM	787	NE	ARG	119	14.226	14.503	114.632	1.00	11.37	A	
ATOM	788	CZ	ARG	119	14.274	15.409	115.601	1.00	9.83	A	

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ATOM    789  NH1 ARG   119      14.607  16.663 115.326  1.00  8.80      A
ATOM    790  NH2 ARG   119      14.003  15.052 116.851  1.00  8.38      A
ATOM    791  C   ARG   119      10.909  12.278 113.012  1.00 13.30      A
ATOM    792  O   ARG   119      10.055  12.134 112.140  1.00 12.33      A
ATOM    793  N   SER   120      10.746  11.819 114.244  1.00 14.08      A
ATOM    794  CA  SER   120       9.478  11.232 114.630  1.00 14.63      A
ATOM    795  CB  SER   120       9.563  10.651 116.037  1.00 13.18      A
ATOM    796  OG  SER   120      10.380   9.500 116.043  1.00 13.75      A
ATOM    797  C   SER   120       8.542  12.434 114.610  1.00 14.70      A
ATOM    798  O   SER   120       8.966  13.556 114.877  1.00 14.22      A
ATOM    799  N   PRO   121       7.263  12.222 114.295  1.00 15.80      A
ATOM    800  CD  PRO   121       6.629  10.969 113.860  1.00 15.88      A
ATOM    801  CA  PRO   121       6.312  13.340 114.253  1.00 16.98      A
ATOM    802  CB  PRO   121       5.037  12.699 113.703  1.00 17.68      A
ATOM    803  CG  PRO   121       5.528  11.476 112.967  1.00 18.94      A
ATOM    804  C   PRO   121       6.036  14.035 115.589  1.00 17.31      A
ATOM    805  O   PRO   121       6.316  13.495 116.662  1.00 17.01      A
ATOM    806  N   ASN   122       5.493  15.249 115.498  1.00 18.27      A
ATOM    807  CA  ASN   122       5.079  16.029 116.659  1.00 19.75      A
ATOM    808  CB  ASN   122       3.899  15.303 117.323  1.00 22.14      A
ATOM    809  CG  ASN   122       2.806  16.243 117.782  1.00 25.67      A
ATOM    810  OD1 ASN   122       2.331  17.090 117.020  1.00 28.24      A
ATOM    811  ND2 ASN   122       2.386  16.089 119.029  1.00 29.36      A
ATOM    812  C   ASN   122       6.137  16.341 117.714  1.00 20.30      A
ATOM    813  O   ASN   122       5.810  16.490 118.889  1.00 19.52      A
ATOM    814  N   GLU   123       7.398  16.443 117.312  1.00 20.21      A
ATOM    815  CA  GLU   123       8.460  16.745 118.267  1.00 21.19      A
ATOM    816  CB  GLU   123       8.341  18.185 118.781  1.00 20.11      A
ATOM    817  CG  GLU   123       8.519  19.249 117.731  1.00 20.41      A
ATOM    818  CD  GLU   123       8.575  20.654 118.319  1.00 21.92      A
ATOM    819  OE1 GLU   123       7.688  21.013 119.133  1.00 18.15      A
ATOM    820  OE2 GLU   123       9.507  21.404 117.951  1.00 21.94      A
ATOM    821  C   GLU   123       8.446  15.806 119.468  1.00 21.37      A
ATOM    822  O   GLU   123       8.632  16.247 120.602  1.00 19.07      A
ATOM    823  N   GLU   124       8.226  14.518 119.233  1.00 22.79      A
ATOM    824  CA  GLU   124       8.210  13.577 120.339  1.00 22.88      A
ATOM    825  CB  GLU   124       7.685  12.215 119.887  1.00 25.26      A
ATOM    826  CG  GLU   124       7.600  11.205 121.033  1.00 30.44      A
ATOM    827  CD  GLU   124       6.924   9.899 120.636  1.00 34.84      A
ATOM    828  OE1 GLU   124       6.827   9.003 121.508  1.00 33.81      A
ATOM    829  OE2 GLU   124       6.494   9.772 119.464  1.00 37.51      A
ATOM    830  C   GLU   124       9.592  13.404 120.964  1.00 22.45      A
ATOM    831  O   GLU   124       9.715  13.235 122.180  1.00 23.30      A
ATOM    832  N   TYR   125      10.635  13.452 120.142  1.00 20.18      A
ATOM    833  CA  TYR   125      11.988  13.269 120.657  1.00 19.15      A
ATOM    834  CB  TYR   125      12.602  11.953 120.150  1.00 17.84      A
ATOM    835  CG  TYR   125      11.805  10.695 120.391  1.00 17.89      A
ATOM    836  CD1 TYR   125      10.791  10.304 119.513  1.00 18.58      A
ATOM    837  CE1 TYR   125      10.086   9.120 119.713  1.00 18.72      A
ATOM    838  CD2 TYR   125      12.090   9.871 121.477  1.00 17.89      A
ATOM    839  CE2 TYR   125      11.395   8.691 121.686  1.00 17.82      A
ATOM    840  CZ  TYR   125      10.398   8.321 120.804  1.00 19.43      A
ATOM    841  OH  TYR   125       9.724   7.142 121.017  1.00 23.55      A
ATOM    842  C   TYR   125      12.941  14.377 120.260  1.00 18.68      A
ATOM    843  O   TYR   125      12.678  15.144 119.338  1.00 20.06      A
ATOM    844  N   THR   126      14.061  14.445 120.971  1.00 18.30      A
ATOM    845  CA  THR   126      15.106  15.402 120.651  1.00 18.04      A
ATOM    846  CB  THR   126      16.063  15.618 121.839  1.00 18.63      A
ATOM    847  OG1 THR   126      16.592  14.356 122.254  1.00 20.05      A
ATOM    848  CG2 THR   126      15.339  16.258 123.014  1.00 18.83      A
ATOM    849  C   THR   126      15.838  14.653 119.537  1.00 17.89      A
ATOM    850  O   THR   126      15.606  13.455 119.355  1.00 16.79      A
ATOM    851  N   TRP   127      16.708  15.322 118.789  1.00 16.50      A
ATOM    852  CA  TRP   127      17.401  14.636 117.711  1.00 16.42      A
ATOM    853  CB  TRP   127      18.198  15.642 116.868  1.00 14.53      A
ATOM    854  CG  TRP   127      19.443  16.133 117.506  1.00 12.21      A
ATOM    855  CD2 TRP   127      20.746  15.554 117.381  1.00 12.40      A
ATOM    856  CE2 TRP   127      21.634  16.350 118.138  1.00 12.89      A
ATOM    857  CE3 TRP   127      21.250  14.436 116.703  1.00 10.82      A
ATOM    858  CD1 TRP   127      19.580  17.225 118.314  1.00 12.48      A
ATOM    859  NE1 TRP   127      20.899  17.365 118.698  1.00 14.38      A
ATOM    860  CZ2 TRP   127      22.997  16.063 118.233  1.00 12.67      A
ATOM    861  CZ3 TRP   127      22.607  14.148 116.800  1.00  8.68      A
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ATOM	862	CH2	TRP	127	23.463	14.959	117.558	1.00	10.75	A
ATOM	863	C	TRP	127	18.318	13.500	118.191	1.00	18.04	A
ATOM	864	O	TRP	127	18.496	12.507	117.491	1.00	17.73	A
ATOM	865	N	GLU	128	18.874	13.639	119.390	1.00	20.55	A
ATOM	866	CA	GLU	128	19.773	12.630	119.954	1.00	22.98	A
ATOM	867	CB	GLU	128	20.449	13.167	121.216	1.00	24.66	A
ATOM	868	CG	GLU	128	21.328	14.375	121.028	1.00	30.86	A
ATOM	869	CD	GLU	128	21.812	14.929	122.359	1.00	34.39	A
ATOM	870	OE1	GLU	128	22.271	14.126	123.204	1.00	36.58	A
ATOM	871	OE2	GLU	128	21.734	16.160	122.562	1.00	36.22	A
ATOM	872	C	GLU	128	19.092	11.322	120.336	1.00	21.59	A
ATOM	873	O	GLU	128	19.744	10.291	120.456	1.00	20.67	A
ATOM	874	N	GLU	129	17.784	11.362	120.539	1.00	22.17	A
ATOM	875	CA	GLU	129	17.073	10.167	120.974	1.00	22.68	A
ATOM	876	CB	GLU	129	16.487	10.426	122.364	1.00	23.27	A
ATOM	877	CG	GLU	129	17.550	10.770	123.392	1.00	28.13	A
ATOM	878	CD	GLU	129	16.965	11.157	124.737	1.00	32.95	A
ATOM	879	OE1	GLU	129	17.752	11.323	125.702	1.00	33.26	A
ATOM	880	OE2	GLU	129	15.724	11.301	124.827	1.00	31.63	A
ATOM	881	C	GLU	129	15.983	9.679	120.035	1.00	20.72	A
ATOM	882	O	GLU	129	15.273	8.728	120.343	1.00	23.09	A
ATOM	883	N	ASP	130	15.862	10.322	118.885	1.00	18.40	A
ATOM	884	CA	ASP	130	14.846	9.945	117.918	1.00	16.36	A
ATOM	885	CB	ASP	130	14.770	11.015	116.828	1.00	15.71	A
ATOM	886	CG	ASP	130	13.495	10.947	116.031	1.00	15.49	A
ATOM	887	OD1	ASP	130	13.044	12.002	115.545	1.00	17.27	A
ATOM	888	OD2	ASP	130	12.950	9.839	115.874	1.00	15.06	A
ATOM	889	C	ASP	130	15.168	8.573	117.326	1.00	15.41	A
ATOM	890	O	ASP	130	16.196	8.377	116.680	1.00	15.65	A
ATOM	891	N	PRO	131	14.287	7.597	117.548	1.00	14.81	A
ATOM	892	CD	PRO	131	12.980	7.675	118.222	1.00	14.52	A
ATOM	893	CA	PRO	131	14.523	6.255	117.018	1.00	15.02	A
ATOM	894	CB	PRO	131	13.348	5.457	117.579	1.00	15.21	A
ATOM	895	CG	PRO	131	12.267	6.478	117.656	1.00	16.02	A
ATOM	896	C	PRO	131	14.607	6.183	115.492	1.00	15.04	A
ATOM	897	O	PRO	131	15.103	5.196	114.943	1.00	12.71	A
ATOM	898	N	LEU	132	14.125	7.224	114.814	1.00	14.88	A
ATOM	899	CA	LEU	132	14.161	7.254	113.354	1.00	14.03	A
ATOM	900	CB	LEU	132	12.947	8.007	112.796	1.00	12.82	A
ATOM	901	CG	LEU	132	11.562	7.434	113.129	1.00	14.44	A
ATOM	902	CD1	LEU	132	10.506	8.271	112.397	1.00	8.97	A
ATOM	903	CD2	LEU	132	11.470	5.950	112.724	1.00	8.90	A
ATOM	904	C	LEU	132	15.446	7.861	112.786	1.00	12.21	A
ATOM	905	O	LEU	132	15.626	7.916	111.573	1.00	11.16	A
ATOM	906	N	ALA	133	16.337	8.321	113.655	1.00	11.83	A
ATOM	907	CA	ALA	133	17.604	8.891	113.186	1.00	11.94	A
ATOM	908	CB	ALA	133	18.447	9.345	114.377	1.00	7.70	A
ATOM	909	C	ALA	133	18.367	7.825	112.373	1.00	12.53	A
ATOM	910	O	ALA	133	18.308	6.637	112.693	1.00	12.95	A
ATOM	911	N	GLY	134	19.074	8.256	111.330	1.00	13.23	A
ATOM	912	CA	GLY	134	19.832	7.328	110.506	1.00	13.31	A
ATOM	913	C	GLY	134	21.314	7.273	110.858	1.00	14.51	A
ATOM	914	O	GLY	134	21.727	7.771	111.910	1.00	12.96	A
ATOM	915	N	ILE	135	22.111	6.685	109.962	1.00	13.27	A
ATOM	916	CA	ILE	135	23.547	6.529	110.158	1.00	10.64	A
ATOM	917	CB	ILE	135	24.211	5.825	108.945	1.00	12.21	A
ATOM	918	CG2	ILE	135	25.728	5.725	109.166	1.00	9.26	A
ATOM	919	CG1	ILE	135	23.606	4.433	108.749	1.00	9.44	A
ATOM	920	CD1	ILE	135	24.194	3.659	107.563	1.00	7.34	A
ATOM	921	C	ILE	135	24.319	7.817	110.429	1.00	11.04	A
ATOM	922	O	ILE	135	25.101	7.868	111.370	1.00	12.98	A
ATOM	923	N	ILE	136	24.117	8.843	109.606	1.00	10.10	A
ATOM	924	CA	ILE	136	24.822	10.109	109.783	1.00	10.16	A
ATOM	925	CB	ILE	136	24.393	11.137	108.709	1.00	9.76	A
ATOM	926	CG2	ILE	136	25.052	12.489	108.966	1.00	7.05	A
ATOM	927	CG1	ILE	136	24.783	10.611	107.327	1.00	8.04	A
ATOM	928	CD1	ILE	136	24.420	11.555	106.177	1.00	8.70	A
ATOM	929	C	ILE	136	24.680	10.734	111.180	1.00	10.98	A
ATOM	930	O	ILE	136	25.673	10.974	111.848	1.00	11.07	A
ATOM	931	N	PRO	137	23.449	11.015	111.637	1.00	12.76	A
ATOM	932	CD	PRO	137	22.118	10.891	111.018	1.00	12.91	A
ATOM	933	CA	PRO	137	23.344	11.609	112.974	1.00	13.27	A
ATOM	934	CB	PRO	137	21.863	11.966	113.079	1.00	12.28	A

ATOM	935	CG	PRO	137	21.210	10.920	112.226	1.00	12.44	A
ATOM	936	C	PRO	137	23.814	10.707	114.117	1.00	13.75	A
ATOM	937	O	PRO	137	24.349	11.191	115.118	1.00	13.93	A
ATOM	938	N	ARG	138	23.616	9.401	113.982	1.00	13.99	A
ATOM	939	CA	ARG	138	24.061	8.490	115.034	1.00	14.63	A
ATOM	940	CB	ARG	138	23.520	7.083	114.788	1.00	11.07	A
ATOM	941	CG	ARG	138	22.026	6.971	115.030	1.00	10.07	A
ATOM	942	CD	ARG	138	21.514	5.574	114.706	1.00	12.89	A
ATOM	943	NE	ARG	138	20.063	5.502	114.816	1.00	14.12	A
ATOM	944	CZ	ARG	138	19.395	5.417	115.961	1.00	16.84	A
ATOM	945	NH1	ARG	138	20.043	5.380	117.123	1.00	17.01	A
ATOM	946	NH2	ARG	138	18.070	5.405	115.943	1.00	16.58	A
ATOM	947	C	ARG	138	25.590	8.479	115.105	1.00	14.82	A
ATOM	948	O	ARG	138	26.175	8.491	116.189	1.00	17.18	A
ATOM	949	N	THR	139	26.227	8.490	113.943	1.00	13.19	A
ATOM	950	CA	THR	139	27.676	8.487	113.864	1.00	14.27	A
ATOM	951	CB	THR	139	28.134	8.347	112.394	1.00	15.10	A
ATOM	952	OG1	THR	139	27.671	7.092	111.877	1.00	16.74	A
ATOM	953	CG2	THR	139	29.663	8.403	112.290	1.00	15.25	A
ATOM	954	C	THR	139	28.315	9.738	114.473	1.00	14.96	A
ATOM	955	O	THR	139	29.268	9.642	115.247	1.00	16.32	A
ATOM	956	N	LEU	140	27.802	10.912	114.128	1.00	13.16	A
ATOM	957	CA	LEU	140	28.374	12.136	114.664	1.00	13.55	A
ATOM	958	CB	LEU	140	27.742	13.351	113.988	1.00	13.68	A
ATOM	959	CG	LEU	140	28.065	13.435	112.489	1.00	15.01	A
ATOM	960	CD1	LEU	140	27.116	14.410	111.824	1.00	15.28	A
ATOM	961	CD2	LEU	140	29.535	13.845	112.286	1.00	12.18	A
ATOM	962	C	LEU	140	28.168	12.200	116.165	1.00	14.55	A
ATOM	963	O	LEU	140	29.031	12.674	116.900	1.00	14.87	A
ATOM	964	N	HIS	141	27.021	11.712	116.621	1.00	15.53	A
ATOM	965	CA	HIS	141	26.715	11.731	118.041	1.00	15.51	A
ATOM	966	CB	HIS	141	25.241	11.359	118.265	1.00	17.50	A
ATOM	967	CG	HIS	141	24.809	11.401	119.698	1.00	19.49	A
ATOM	968	CD2	HIS	141	24.144	12.349	120.400	1.00	20.09	A
ATOM	969	ND1	HIS	141	25.057	10.373	120.584	1.00	22.94	A
ATOM	970	CE1	HIS	141	24.561	10.686	121.769	1.00	21.94	A
ATOM	971	NE2	HIS	141	24.002	11.880	121.683	1.00	21.59	A
ATOM	972	C	HIS	141	27.638	10.772	118.787	1.00	14.45	A
ATOM	973	O	HIS	141	28.133	11.094	119.864	1.00	12.82	A
ATOM	974	N	GLN	142	27.893	9.606	118.202	1.00	12.87	A
ATOM	975	CA	GLN	142	28.753	8.627	118.852	1.00	14.02	A
ATOM	976	CB	GLN	142	28.542	7.248	118.239	1.00	13.39	A
ATOM	977	CG	GLN	142	27.299	6.545	118.741	1.00	20.05	A
ATOM	978	CD	GLN	142	27.237	6.484	120.262	1.00	21.32	A
ATOM	979	OE1	GLN	142	26.660	7.361	120.910	1.00	21.37	A
ATOM	980	NE2	GLN	142	27.850	5.454	120.837	1.00	19.74	A
ATOM	981	C	GLN	142	30.243	8.963	118.862	1.00	13.74	A
ATOM	982	O	GLN	142	30.961	8.535	119.759	1.00	14.17	A
ATOM	983	N	ILE	143	30.713	9.709	117.870	1.00	13.21	A
ATOM	984	CA	ILE	143	32.119	10.087	117.826	1.00	13.39	A
ATOM	985	CB	ILE	143	32.435	10.932	116.576	1.00	11.43	A
ATOM	986	CG2	ILE	143	33.847	11.507	116.678	1.00	13.15	A
ATOM	987	CG1	ILE	143	32.282	10.068	115.324	1.00	9.90	A
ATOM	988	CD1	ILE	143	32.437	10.844	114.012	1.00	8.46	A
ATOM	989	C	ILE	143	32.454	10.897	119.082	1.00	14.99	A
ATOM	990	O	ILE	143	33.473	10.660	119.724	1.00	13.04	A
ATOM	991	N	PHE	144	31.581	11.848	119.419	1.00	17.68	A
ATOM	992	CA	PHE	144	31.741	12.694	120.599	1.00	20.78	A
ATOM	993	CB	PHE	144	30.771	13.882	120.548	1.00	17.56	A
ATOM	994	CG	PHE	144	31.153	14.924	119.549	1.00	18.09	A
ATOM	995	CD1	PHE	144	32.205	15.796	119.809	1.00	18.10	A
ATOM	996	CD2	PHE	144	30.492	15.013	118.327	1.00	17.52	A
ATOM	997	CE1	PHE	144	32.596	16.740	118.864	1.00	19.03	A
ATOM	998	CE2	PHE	144	30.873	15.949	117.371	1.00	16.50	A
ATOM	999	CZ	PHE	144	31.926	16.817	117.639	1.00	18.32	A
ATOM	1000	C	PHE	144	31.481	11.908	121.877	1.00	24.06	A
ATOM	1001	O	PHE	144	32.059	12.203	122.917	1.00	25.61	A
ATOM	1002	N	GLU	145	30.596	10.924	121.801	1.00	28.05	A
ATOM	1003	CA	GLU	145	30.270	10.113	122.963	1.00	32.18	A
ATOM	1004	CB	GLU	145	29.052	9.233	122.660	1.00	34.92	A
ATOM	1005	CG	GLU	145	28.382	8.616	123.877	1.00	41.48	A
ATOM	1006	CD	GLU	145	27.459	9.586	124.604	1.00	46.68	A
ATOM	1007	OE1	GLU	145	26.808	9.154	125.583	1.00	48.85	A

ATOM	1008	OE2	GLU	145	27.379	10.772	124.205	1.00	48.27	A
ATOM	1009	C	GLU	145	31.472	9.234	123.300	1.00	33.53	A
ATOM	1010	O	GLU	145	31.796	9.031	124.465	1.00	35.14	A
ATOM	1011	N	LYS	146	32.139	8.727	122.272	1.00	33.94	A
ATOM	1012	CA	LYS	146	33.289	7.857	122.460	1.00	35.62	A
ATOM	1013	CB	LYS	146	33.493	6.982	121.218	1.00	35.76	A
ATOM	1014	CG	LYS	146	32.398	5.949	120.990	1.00	38.40	A
ATOM	1015	CD	LYS	146	32.750	5.000	119.853	1.00	39.00	A
ATOM	1016	CE	LYS	146	31.822	3.804	119.842	1.00	40.55	A
ATOM	1017	NZ	LYS	146	32.108	2.871	118.719	1.00	42.99	A
ATOM	1018	C	LYS	146	34.600	8.572	122.781	1.00	37.30	A
ATOM	1019	O	LYS	146	35.279	8.224	123.746	1.00	38.30	A
ATOM	1020	N	LEU	147	34.959	9.567	121.978	1.00	37.75	A
ATOM	1021	CA	LEU	147	36.212	10.286	122.182	1.00	39.45	A
ATOM	1022	CB	LEU	147	36.611	11.013	120.894	1.00	36.70	A
ATOM	1023	CG	LEU	147	36.769	10.134	119.652	1.00	34.99	A
ATOM	1024	CD1	LEU	147	37.244	10.979	118.483	1.00	32.76	A
ATOM	1025	CD2	LEU	147	37.754	9.012	119.940	1.00	33.24	A
ATOM	1026	C	LEU	147	36.250	11.268	123.355	1.00	41.40	A
ATOM	1027	O	LEU	147	37.329	11.653	123.803	1.00	41.57	A
ATOM	1028	N	THR	148	35.091	11.681	123.855	1.00	43.50	A
ATOM	1029	CA	THR	148	35.078	12.613	124.972	1.00	46.76	A
ATOM	1030	CB	THR	148	33.735	13.379	125.068	1.00	46.73	A
ATOM	1031	OG1	THR	148	33.559	14.194	123.901	1.00	45.09	A
ATOM	1032	CG2	THR	148	33.717	14.274	126.299	1.00	45.59	A
ATOM	1033	C	THR	148	35.327	11.848	126.266	1.00	50.09	A
ATOM	1034	O	THR	148	36.050	12.321	127.149	1.00	50.49	A
ATOM	1035	N	ASP	149	34.734	10.660	126.367	1.00	53.41	A
ATOM	1036	CA	ASP	149	34.899	9.812	127.545	1.00	56.45	A
ATOM	1037	CB	ASP	149	34.094	8.515	127.395	1.00	57.31	A
ATOM	1038	CG	ASP	149	32.677	8.641	127.926	1.00	59.22	A
ATOM	1039	OD1	ASP	149	32.519	9.073	129.090	1.00	59.37	A
ATOM	1040	OD2	ASP	149	31.723	8.302	127.191	1.00	59.44	A
ATOM	1041	C	ASP	149	36.365	9.468	127.778	1.00	57.60	A
ATOM	1042	O	ASP	149	36.948	9.837	128.800	1.00	57.84	A
ATOM	1043	N	ASN	150	36.955	8.756	126.824	1.00	58.66	A
ATOM	1044	CA	ASN	150	38.354	8.366	126.919	1.00	59.63	A
ATOM	1045	CB	ASN	150	38.699	7.388	125.793	1.00	62.63	A
ATOM	1046	CG	ASN	150	37.845	6.129	125.832	1.00	65.36	A
ATOM	1047	OD1	ASN	150	37.880	5.366	126.803	1.00	66.45	A
ATOM	1048	ND2	ASN	150	37.070	5.908	124.774	1.00	66.13	A
ATOM	1049	C	ASN	150	39.248	9.598	126.833	1.00	58.25	A
ATOM	1050	O	ASN	150	38.814	10.657	126.382	1.00	58.50	A
ATOM	1051	N	GLY	151	40.492	9.459	127.279	1.00	56.63	A
ATOM	1052	CA	GLY	151	41.416	10.579	127.233	1.00	55.03	A
ATOM	1053	C	GLY	151	41.915	10.801	125.820	1.00	53.26	A
ATOM	1054	O	GLY	151	42.983	10.307	125.449	1.00	52.83	A
ATOM	1055	N	THR	152	41.149	11.551	125.029	1.00	50.83	A
ATOM	1056	CA	THR	152	41.519	11.806	123.643	1.00	47.73	A
ATOM	1057	CB	THR	152	40.763	10.858	122.680	1.00	47.39	A
ATOM	1058	OG1	THR	152	40.890	9.502	123.127	1.00	48.20	A
ATOM	1059	CG2	THR	152	41.326	10.975	121.271	1.00	45.61	A
ATOM	1060	C	THR	152	41.237	13.230	123.180	1.00	46.24	A
ATOM	1061	O	THR	152	40.163	13.775	123.425	1.00	46.24	A
ATOM	1062	N	GLU	153	42.217	13.828	122.510	1.00	43.69	A
ATOM	1063	CA	GLU	153	42.066	15.165	121.957	1.00	41.25	A
ATOM	1064	CB	GLU	153	43.386	15.926	122.014	1.00	42.93	A
ATOM	1065	CG	GLU	153	43.815	16.330	123.407	1.00	46.50	A
ATOM	1066	CD	GLU	153	45.193	16.952	123.421	1.00	48.91	A
ATOM	1067	OE1	GLU	153	46.181	16.219	123.196	1.00	49.46	A
ATOM	1068	OE2	GLU	153	45.288	18.177	123.649	1.00	52.22	A
ATOM	1069	C	GLU	153	41.677	14.898	120.508	1.00	38.96	A
ATOM	1070	O	GLU	153	42.232	13.998	119.874	1.00	38.36	A
ATOM	1071	N	PHE	154	40.730	15.665	119.980	1.00	35.01	A
ATOM	1072	CA	PHE	154	40.289	15.434	118.611	1.00	30.73	A
ATOM	1073	CB	PHE	154	39.416	14.177	118.574	1.00	27.60	A
ATOM	1074	CG	PHE	154	38.102	14.340	119.282	1.00	24.32	A
ATOM	1075	CD1	PHE	154	36.965	14.742	118.585	1.00	22.22	A
ATOM	1076	CD2	PHE	154	38.009	14.130	120.652	1.00	24.15	A
ATOM	1077	CE1	PHE	154	35.751	14.929	119.246	1.00	22.43	A
ATOM	1078	CE2	PHE	154	36.797	14.316	121.327	1.00	24.33	A
ATOM	1079	CZ	PHE	154	35.664	14.718	120.618	1.00	23.63	A
ATOM	1080	C	PHE	154	39.498	16.590	118.024	1.00	28.48	A

ATOM	1081	O	PHE	154	38.921	17.402	118.744	1.00	27.87	A
ATOM	1082	N	SER	155	39.474	16.653	116.702	1.00	26.86	A
ATOM	1083	CA	SER	155	38.713	17.676	116.006	1.00	25.68	A
ATOM	1084	CB	SER	155	39.635	18.708	115.347	1.00	24.22	A
ATOM	1085	OG	SER	155	40.401	18.131	114.309	1.00	25.09	A
ATOM	1086	C	SER	155	37.920	16.925	114.947	1.00	26.10	A
ATOM	1087	O	SER	155	38.402	15.937	114.380	1.00	26.26	A
ATOM	1088	N	VAL	156	36.697	17.377	114.700	1.00	25.35	A
ATOM	1089	CA	VAL	156	35.836	16.741	113.712	1.00	23.66	A
ATOM	1090	CB	VAL	156	34.549	16.202	114.371	1.00	22.75	A
ATOM	1091	CG1	VAL	156	33.671	15.499	113.331	1.00	20.72	A
ATOM	1092	CG2	VAL	156	34.910	15.257	115.497	1.00	20.01	A
ATOM	1093	C	VAL	156	35.447	17.733	112.622	1.00	24.01	A
ATOM	1094	O	VAL	156	34.960	18.832	112.916	1.00	24.09	A
ATOM	1095	N	LYS	157	35.679	17.344	111.369	1.00	21.25	A
ATOM	1096	CA	LYS	157	35.332	18.172	110.220	1.00	20.34	A
ATOM	1097	CB	LYS	157	36.559	18.467	109.347	1.00	24.12	A
ATOM	1098	CG	LYS	157	37.755	19.140	110.028	1.00	28.05	A
ATOM	1099	CD	LYS	157	37.474	20.581	110.410	1.00	31.98	A
ATOM	1100	CE	LYS	157	38.755	21.314	110.845	1.00	35.17	A
ATOM	1101	NZ	LYS	157	39.737	21.545	109.726	1.00	35.98	A
ATOM	1102	C	LYS	157	34.333	17.380	109.382	1.00	19.05	A
ATOM	1103	O	LYS	157	34.475	16.166	109.209	1.00	18.10	A
ATOM	1104	N	VAL	158	33.315	18.057	108.865	1.00	15.97	A
ATOM	1105	CA	VAL	158	32.340	17.380	108.025	1.00	14.22	A
ATOM	1106	CB	VAL	158	30.941	17.281	108.690	1.00	12.88	A
ATOM	1107	CG1	VAL	158	31.014	16.411	109.931	1.00	10.13	A
ATOM	1108	CG2	VAL	158	30.419	18.651	109.031	1.00	13.23	A
ATOM	1109	C	VAL	158	32.221	18.106	106.706	1.00	13.72	A
ATOM	1110	O	VAL	158	32.469	19.300	106.610	1.00	14.66	A
ATOM	1111	N	SER	159	31.845	17.373	105.677	1.00	14.86	A
ATOM	1112	CA	SER	159	31.702	17.955	104.362	1.00	16.10	A
ATOM	1113	CB	SER	159	33.034	17.844	103.618	1.00	17.14	A
ATOM	1114	OG	SER	159	32.904	18.263	102.279	1.00	23.83	A
ATOM	1115	C	SER	159	30.609	17.186	103.642	1.00	15.89	A
ATOM	1116	O	SER	159	30.477	15.976	103.822	1.00	15.28	A
ATOM	1117	N	LEU	160	29.820	17.890	102.838	1.00	15.69	A
ATOM	1118	CA	LEU	160	28.728	17.268	102.098	1.00	15.26	A
ATOM	1119	CB	LEU	160	27.388	17.679	102.715	1.00	15.28	A
ATOM	1120	CG	LEU	160	26.121	17.071	102.104	1.00	15.37	A
ATOM	1121	CD1	LEU	160	26.236	15.559	102.087	1.00	12.97	A
ATOM	1122	CD2	LEU	160	24.904	17.517	102.904	1.00	14.38	A
ATOM	1123	C	LEU	160	28.799	17.689	100.640	1.00	15.74	A
ATOM	1124	O	LEU	160	28.331	18.766	100.263	1.00	15.17	A
ATOM	1125	N	LEU	161	29.394	16.822	99.829	1.00	15.44	A
ATOM	1126	CA	LEU	161	29.577	17.052	98.401	1.00	15.04	A
ATOM	1127	CB	LEU	161	30.923	16.472	97.968	1.00	16.39	A
ATOM	1128	CG	LEU	161	31.753	17.038	96.815	1.00	19.66	A
ATOM	1129	CD1	LEU	161	32.749	15.955	96.386	1.00	20.66	A
ATOM	1130	CD2	LEU	161	30.887	17.437	95.641	1.00	20.16	A
ATOM	1131	C	LEU	161	28.470	16.311	97.680	1.00	15.70	A
ATOM	1132	O	LEU	161	28.200	15.161	97.989	1.00	17.10	A
ATOM	1133	N	GLU	162	27.829	16.952	96.713	1.00	15.78	A
ATOM	1134	CA	GLU	162	26.763	16.286	95.984	1.00	13.96	A
ATOM	1135	CB	GLU	162	25.413	16.834	96.428	1.00	14.46	A
ATOM	1136	CG	GLU	162	25.218	16.645	97.928	1.00	17.99	A
ATOM	1137	CD	GLU	162	23.781	16.776	98.372	1.00	18.53	A
ATOM	1138	OE1	GLU	162	23.532	16.663	99.588	1.00	20.86	A
ATOM	1139	OE2	GLU	162	22.902	16.984	97.513	1.00	17.99	A
ATOM	1140	C	GLU	162	26.948	16.403	94.489	1.00	12.56	A
ATOM	1141	O	GLU	162	27.425	17.414	93.985	1.00	12.95	A
ATOM	1142	N	ILE	163	26.575	15.346	93.782	1.00	11.75	A
ATOM	1143	CA	ILE	163	26.736	15.303	92.340	1.00	11.19	A
ATOM	1144	CB	ILE	163	27.588	14.077	91.941	1.00	10.80	A
ATOM	1145	CG2	ILE	163	27.790	14.044	90.436	1.00	9.29	A
ATOM	1146	CG1	ILE	163	28.927	14.121	92.681	1.00	10.31	A
ATOM	1147	CD1	ILE	163	29.667	12.777	92.718	1.00	12.19	A
ATOM	1148	C	ILE	163	25.393	15.238	91.626	1.00	11.81	A
ATOM	1149	O	ILE	163	24.524	14.441	91.985	1.00	13.50	A
ATOM	1150	N	TYR	164	25.228	16.089	90.620	1.00	10.80	A
ATOM	1151	CA	TYR	164	24.011	16.125	89.826	1.00	11.96	A
ATOM	1152	CB	TYR	164	23.038	17.194	90.353	1.00	11.56	A
ATOM	1153	CG	TYR	164	21.746	17.240	89.573	1.00	10.77	A

ATOM	1154	CD1	TYR	164	21.639	18.005	88.408	1.00	9.75	A
ATOM	1155	CE1	TYR	164	20.479	17.991	87.638	1.00	8.60	A
ATOM	1156	CD2	TYR	164	20.653	16.457	89.954	1.00	8.92	A
ATOM	1157	CE2	TYR	164	19.483	16.428	89.187	1.00	9.51	A
ATOM	1158	CZ	TYR	164	19.405	17.197	88.031	1.00	10.37	A
ATOM	1159	OH	TYR	164	18.264	17.167	87.261	1.00	9.00	A
ATOM	1160	C	TYR	164	24.415	16.443	88.395	1.00	12.68	A
ATOM	1161	O	TYR	164	25.048	17.468	88.131	1.00	13.49	A
ATOM	1162	N	ASN	165	24.075	15.550	87.478	1.00	12.65	A
ATOM	1163	CA	ASN	165	24.410	15.745	86.078	1.00	14.45	A
ATOM	1164	CB	ASN	165	23.541	16.864	85.515	1.00	18.24	A
ATOM	1165	CG	ASN	165	23.498	16.869	84.010	1.00	24.46	A
ATOM	1166	OD1	ASN	165	23.396	15.817	83.374	1.00	29.01	A
ATOM	1167	ND2	ASN	165	23.556	18.061	83.422	1.00	27.99	A
ATOM	1168	C	ASN	165	25.903	16.069	85.930	1.00	14.74	A
ATOM	1169	O	ASN	165	26.290	16.972	85.184	1.00	13.82	A
ATOM	1170	N	GLU	166	26.729	15.321	86.663	1.00	13.32	A
ATOM	1171	CA	GLU	166	28.178	15.475	86.645	1.00	13.84	A
ATOM	1172	CB	GLU	166	28.730	15.118	85.265	1.00	11.37	A
ATOM	1173	CG	GLU	166	28.676	13.635	84.952	1.00	13.48	A
ATOM	1174	CD	GLU	166	29.270	12.781	86.069	1.00	15.85	A
ATOM	1175	OE1	GLU	166	28.518	12.411	86.995	1.00	14.50	A
ATOM	1176	OE2	GLU	166	30.491	12.490	86.022	1.00	14.74	A
ATOM	1177	C	GLU	166	28.724	16.835	87.067	1.00	15.33	A
ATOM	1178	O	GLU	166	29.809	17.229	86.650	1.00	16.01	A
ATOM	1179	N	GLU	167	27.970	17.555	87.885	1.00	16.84	A
ATOM	1180	CA	GLU	167	28.415	18.850	88.381	1.00	16.72	A
ATOM	1181	CB	GLU	167	27.403	19.949	88.052	1.00	19.43	A
ATOM	1182	CG	GLU	167	27.235	20.216	86.570	1.00	23.50	A
ATOM	1183	CD	GLU	167	26.307	21.388	86.309	1.00	28.67	A
ATOM	1184	OE1	GLU	167	25.176	21.382	86.846	1.00	32.20	A
ATOM	1185	OE2	GLU	167	26.707	22.316	85.571	1.00	31.83	A
ATOM	1186	C	GLU	167	28.522	18.685	89.888	1.00	15.13	A
ATOM	1187	O	GLU	167	27.773	17.908	90.480	1.00	15.63	A
ATOM	1188	N	LEU	168	29.449	19.408	90.501	1.00	12.84	A
ATOM	1189	CA	LEU	168	29.672	19.312	91.939	1.00	12.94	A
ATOM	1190	CB	LEU	168	31.171	19.220	92.217	1.00	14.17	A
ATOM	1191	CG	LEU	168	31.859	17.853	92.232	1.00	18.45	A
ATOM	1192	CD1	LEU	168	31.289	16.947	91.164	1.00	19.30	A
ATOM	1193	CD2	LEU	168	33.366	18.058	92.047	1.00	18.21	A
ATOM	1194	C	LEU	168	29.080	20.467	92.732	1.00	11.51	A
ATOM	1195	O	LEU	168	29.228	21.631	92.357	1.00	12.03	A
ATOM	1196	N	PHE	169	28.415	20.138	93.834	1.00	8.76	A
ATOM	1197	CA	PHE	169	27.812	21.152	94.682	1.00	10.79	A
ATOM	1198	CB	PHE	169	26.286	21.155	94.543	1.00	8.69	A
ATOM	1199	CG	PHE	169	25.804	21.329	93.127	1.00	9.29	A
ATOM	1200	CD1	PHE	169	25.568	20.219	92.314	1.00	8.53	A
ATOM	1201	CD2	PHE	169	25.605	22.595	92.598	1.00	7.95	A
ATOM	1202	CE1	PHE	169	25.140	20.372	90.996	1.00	9.35	A
ATOM	1203	CE2	PHE	169	25.178	22.762	91.284	1.00	7.75	A
ATOM	1204	CZ	PHE	169	24.945	21.648	90.479	1.00	9.59	A
ATOM	1205	C	PHE	169	28.187	20.923	96.138	1.00	12.65	A
ATOM	1206	O	PHE	169	28.319	19.788	96.593	1.00	13.12	A
ATOM	1207	N	ASP	170	28.369	22.027	96.850	1.00	12.78	A
ATOM	1208	CA	ASP	170	28.724	22.018	98.253	1.00	13.35	A
ATOM	1209	CB	ASP	170	29.817	23.060	98.502	1.00	12.29	A
ATOM	1210	CG	ASP	170	30.300	23.072	99.931	1.00	13.08	A
ATOM	1211	OD1	ASP	170	29.577	22.566	100.817	1.00	14.08	A
ATOM	1212	OD2	ASP	170	31.404	23.598	100.176	1.00	15.39	A
ATOM	1213	C	ASP	170	27.456	22.413	99.001	1.00	15.21	A
ATOM	1214	O	ASP	170	27.086	23.588	99.003	1.00	13.76	A
ATOM	1215	N	LEU	171	26.797	21.445	99.635	1.00	16.64	A
ATOM	1216	CA	LEU	171	25.563	21.722	100.365	1.00	19.47	A
ATOM	1217	CB	LEU	171	24.650	20.483	100.376	1.00	18.16	A
ATOM	1218	CG	LEU	171	23.677	20.315	99.200	1.00	20.70	A
ATOM	1219	CD1	LEU	171	22.739	21.515	99.130	1.00	21.59	A
ATOM	1220	CD2	LEU	171	24.436	20.192	97.900	1.00	19.74	A
ATOM	1221	C	LEU	171	25.724	22.233	101.794	1.00	21.95	A
ATOM	1222	O	LEU	171	24.747	22.282	102.536	1.00	24.93	A
ATOM	1223	N	LEU	172	26.931	22.618	102.197	1.00	24.33	A
ATOM	1224	CA	LEU	172	27.108	23.129	103.558	1.00	25.95	A
ATOM	1225	CB	LEU	172	28.101	22.267	104.353	1.00	22.64	A
ATOM	1226	CG	LEU	172	27.683	20.835	104.713	1.00	21.08	A

ATOM	1227	CD1	LEU	172	28.747	20.208	105.584	1.00	19.49	A
ATOM	1228	CD2	LEU	172	26.353	20.821	105.450	1.00	20.02	A
ATOM	1229	C	LEU	172	27.550	24.592	103.579	1.00	28.46	A
ATOM	1230	O	LEU	172	27.222	25.328	104.512	1.00	33.47	A
ATOM	1231	N	ASN	173	28.280	25.020	102.557	1.00	27.52	A
ATOM	1232	CA	ASN	173	28.733	26.404	102.479	1.00	28.63	A
ATOM	1233	CB	ASN	173	29.491	26.621	101.166	1.00	28.72	A
ATOM	1234	CG	ASN	173	30.022	28.037	101.013	1.00	30.51	A
ATOM	1235	OD1	ASN	173	30.709	28.350	100.038	1.00	32.23	A
ATOM	1236	ND2	ASN	173	29.709	28.898	101.969	1.00	31.50	A
ATOM	1237	C	ASN	173	27.514	27.331	102.555	1.00	30.66	A
ATOM	1238	O	ASN	173	26.639	27.296	101.688	1.00	30.81	A
ATOM	1239	N	PRO	174	27.434	28.164	103.602	1.00	32.10	A
ATOM	1240	CD	PRO	174	28.196	28.086	104.862	1.00	32.35	A
ATOM	1241	CA	PRO	174	26.298	29.076	103.741	1.00	34.00	A
ATOM	1242	CB	PRO	174	26.085	29.107	105.243	1.00	33.56	A
ATOM	1243	CG	PRO	174	27.500	29.119	105.740	1.00	33.25	A
ATOM	1244	C	PRO	174	26.566	30.469	103.179	1.00	35.77	A
ATOM	1245	O	PRO	174	26.014	31.452	103.667	1.00	38.93	A
ATOM	1246	N	SER	175	27.404	30.557	102.155	1.00	36.48	A
ATOM	1247	CA	SER	175	27.734	31.848	101.568	1.00	36.56	A
ATOM	1248	CB	SER	175	29.104	32.312	102.064	1.00	36.53	A
ATOM	1249	OG	SER	175	29.142	32.334	103.481	1.00	38.61	A
ATOM	1250	C	SER	175	27.746	31.745	100.059	1.00	36.99	A
ATOM	1251	O	SER	175	28.234	32.639	99.366	1.00	37.49	A
ATOM	1252	N	SER	176	27.226	30.631	99.560	1.00	37.22	A
ATOM	1253	CA	SER	176	27.142	30.385	98.125	1.00	38.02	A
ATOM	1254	CB	SER	176	28.296	29.483	97.662	1.00	37.78	A
ATOM	1255	OG	SER	176	28.200	28.177	98.213	1.00	37.44	A
ATOM	1256	C	SER	176	25.807	29.699	97.862	1.00	37.53	A
ATOM	1257	O	SER	176	25.277	29.016	98.734	1.00	37.34	A
ATOM	1258	N	ASP	177	25.248	29.891	96.676	1.00	38.02	A
ATOM	1259	CA	ASP	177	23.983	29.243	96.366	1.00	39.18	A
ATOM	1260	CB	ASP	177	23.012	30.229	95.704	1.00	41.03	A
ATOM	1261	CG	ASP	177	23.585	30.879	94.466	1.00	42.23	A
ATOM	1262	OD1	ASP	177	23.936	30.156	93.511	1.00	43.11	A
ATOM	1263	OD2	ASP	177	23.679	32.122	94.447	1.00	44.29	A
ATOM	1264	C	ASP	177	24.219	28.031	95.471	1.00	38.57	A
ATOM	1265	O	ASP	177	25.274	27.910	94.849	1.00	37.31	A
ATOM	1266	N	VAL	178	23.232	27.141	95.415	1.00	38.30	A
ATOM	1267	CA	VAL	178	23.329	25.918	94.626	1.00	38.53	A
ATOM	1268	CB	VAL	178	22.091	25.018	94.830	1.00	38.67	A
ATOM	1269	CG1	VAL	178	22.040	24.532	96.266	1.00	38.55	A
ATOM	1270	CG2	VAL	178	20.828	25.780	94.472	1.00	38.63	A
ATOM	1271	C	VAL	178	23.526	26.111	93.129	1.00	38.49	A
ATOM	1272	O	VAL	178	23.589	25.138	92.385	1.00	39.24	A
ATOM	1273	N	SER	179	23.618	27.357	92.683	1.00	38.10	A
ATOM	1274	CA	SER	179	23.823	27.626	91.268	1.00	37.56	A
ATOM	1275	CB	SER	179	23.265	29.000	90.905	1.00	39.68	A
ATOM	1276	OG	SER	179	21.942	29.155	91.390	1.00	45.54	A
ATOM	1277	C	SER	179	25.318	27.594	90.981	1.00	36.56	A
ATOM	1278	O	SER	179	25.740	27.516	89.828	1.00	37.57	A
ATOM	1279	N	GLU	180	26.112	27.663	92.044	1.00	34.30	A
ATOM	1280	CA	GLU	180	27.566	27.651	91.938	1.00	34.69	A
ATOM	1281	CB	GLU	180	28.173	28.564	93.018	1.00	36.86	A
ATOM	1282	CG	GLU	180	27.906	30.055	92.767	1.00	41.33	A
ATOM	1283	CD	GLU	180	28.262	30.958	93.945	1.00	42.95	A
ATOM	1284	OE1	GLU	180	27.629	30.832	95.017	1.00	43.98	A
ATOM	1285	OE2	GLU	180	29.174	31.798	93.795	1.00	44.03	A
ATOM	1286	C	GLU	180	28.147	26.241	92.048	1.00	32.62	A
ATOM	1287	O	GLU	180	28.084	25.614	93.104	1.00	31.99	A
ATOM	1288	N	ARG	181	28.706	25.745	90.951	1.00	30.63	A
ATOM	1289	CA	ARG	181	29.292	24.415	90.941	1.00	30.51	A
ATOM	1290	CB	ARG	181	29.050	23.739	89.587	1.00	34.25	A
ATOM	1291	CG	ARG	181	29.575	24.493	88.379	1.00	40.52	A
ATOM	1292	CD	ARG	181	29.025	23.901	87.069	1.00	46.73	A
ATOM	1293	NE	ARG	181	29.587	22.592	86.721	1.00	50.11	A
ATOM	1294	CZ	ARG	181	30.818	22.400	86.251	1.00	52.44	A
ATOM	1295	NH1	ARG	181	31.629	23.435	86.070	1.00	53.59	A
ATOM	1296	NH2	ARG	181	31.236	21.173	85.951	1.00	52.52	A
ATOM	1297	C	ARG	181	30.781	24.480	91.249	1.00	28.82	A
ATOM	1298	O	ARG	181	31.438	25.483	90.979	1.00	29.29	A
ATOM	1299	N	LEU	182	31.308	23.408	91.829	1.00	25.57	A

ATOM	1300	CA	LEU	182	32.718	23.348	92.182	1.00	21.92	A
ATOM	1301	CB	LEU	182	32.899	22.553	93.471	1.00	20.02	A
ATOM	1302	CG	LEU	182	32.155	23.087	94.700	1.00	20.20	A
ATOM	1303	CD1	LEU	182	32.161	22.044	95.812	1.00	17.99	A
ATOM	1304	CD2	LEU	182	32.802	24.379	95.159	1.00	16.82	A
ATOM	1305	C	LEU	182	33.515	22.696	91.069	1.00	22.08	A
ATOM	1306	O	LEU	182	32.960	21.949	90.257	1.00	19.82	A
ATOM	1307	N	GLN	183	34.814	23.000	91.028	1.00	22.61	A
ATOM	1308	CA	GLN	183	35.726	22.435	90.034	1.00	20.55	A
ATOM	1309	CB	GLN	183	36.702	23.488	89.523	1.00	22.39	A
ATOM	1310	CG	GLN	183	36.100	24.557	88.652	1.00	28.44	A
ATOM	1311	CD	GLN	183	36.981	25.799	88.593	1.00	32.88	A
ATOM	1312	OE1	GLN	183	37.054	26.572	89.557	1.00	34.28	A
ATOM	1313	NE2	GLN	183	37.664	25.989	87.468	1.00	33.10	A
ATOM	1314	C	GLN	183	36.518	21.327	90.702	1.00	19.22	A
ATOM	1315	O	GLN	183	36.795	21.390	91.897	1.00	18.40	A
ATOM	1316	N	MET	184	36.902	20.330	89.915	1.00	18.69	A
ATOM	1317	CA	MET	184	37.646	19.191	90.416	1.00	19.64	A
ATOM	1318	CB	MET	184	36.747	17.951	90.361	1.00	21.90	A
ATOM	1319	CG	MET	184	37.304	16.701	91.011	1.00	25.13	A
ATOM	1320	SD	MET	184	36.147	15.306	90.921	1.00	31.12	A
ATOM	1321	CE	MET	184	36.591	14.620	89.352	1.00	23.65	A
ATOM	1322	C	MET	184	38.897	18.983	89.568	1.00	21.60	A
ATOM	1323	O	MET	184	38.840	19.035	88.341	1.00	21.33	A
ATOM	1324	N	PHE	185	40.026	18.750	90.230	1.00	23.48	A
ATOM	1325	CA	PHE	185	41.299	18.531	89.544	1.00	25.16	A
ATOM	1326	CB	PHE	185	42.231	19.736	89.709	1.00	25.59	A
ATOM	1327	CG	PHE	185	41.595	21.064	89.414	1.00	25.42	A
ATOM	1328	CD1	PHE	185	40.791	21.691	90.360	1.00	23.63	A
ATOM	1329	CD2	PHE	185	41.857	21.718	88.211	1.00	26.39	A
ATOM	1330	CE1	PHE	185	40.261	22.956	90.124	1.00	24.23	A
ATOM	1331	CE2	PHE	185	41.332	22.987	87.961	1.00	27.17	A
ATOM	1332	CZ	PHE	185	40.533	23.609	88.921	1.00	25.70	A
ATOM	1333	C	PHE	185	42.002	17.326	90.149	1.00	26.03	A
ATOM	1334	O	PHE	185	41.709	16.937	91.275	1.00	25.54	A
ATOM	1335	N	ASP	186	42.941	16.743	89.414	1.00	29.33	A
ATOM	1336	CA	ASP	186	43.692	15.603	89.930	1.00	33.38	A
ATOM	1337	CB	ASP	186	44.461	14.913	88.801	1.00	35.26	A
ATOM	1338	CG	ASP	186	43.546	14.212	87.816	1.00	37.12	A
ATOM	1339	OD1	ASP	186	43.644	14.505	86.603	1.00	37.66	A
ATOM	1340	OD2	ASP	186	42.733	13.368	88.257	1.00	36.31	A
ATOM	1341	C	ASP	186	44.675	16.117	90.977	1.00	35.30	A
ATOM	1342	O	ASP	186	45.167	17.238	90.865	1.00	35.53	A
ATOM	1343	N	ASP	187	44.959	15.313	91.996	1.00	38.26	A
ATOM	1344	CA	ASP	187	45.890	15.739	93.037	1.00	43.31	A
ATOM	1345	CB	ASP	187	45.489	15.138	94.385	1.00	42.12	A
ATOM	1346	CG	ASP	187	46.217	15.784	95.546	1.00	42.51	A
ATOM	1347	OD1	ASP	187	45.755	15.631	96.696	1.00	42.87	A
ATOM	1348	OD2	ASP	187	47.252	16.442	95.307	1.00	41.23	A
ATOM	1349	C	ASP	187	47.307	15.318	92.665	1.00	46.67	A
ATOM	1350	O	ASP	187	47.644	14.138	92.719	1.00	48.15	A
ATOM	1351	N	PRO	188	48.160	16.283	92.286	1.00	50.27	A
ATOM	1352	CD	PRO	188	47.945	17.735	92.408	1.00	50.91	A
ATOM	1353	CA	PRO	188	49.548	15.996	91.897	1.00	53.10	A
ATOM	1354	CB	PRO	188	50.107	17.376	91.561	1.00	52.20	A
ATOM	1355	CG	PRO	188	49.364	18.263	92.503	1.00	52.65	A
ATOM	1356	C	PRO	188	50.366	15.279	92.966	1.00	55.80	A
ATOM	1357	O	PRO	188	51.319	14.568	92.650	1.00	56.91	A
ATOM	1358	N	ARG	189	49.996	15.466	94.228	1.00	58.59	A
ATOM	1359	CA	ARG	189	50.703	14.812	95.321	1.00	61.67	A
ATOM	1360	CB	ARG	189	50.294	15.428	96.658	1.00	63.13	A
ATOM	1361	CG	ARG	189	50.839	16.823	96.881	1.00	65.91	A
ATOM	1362	CD	ARG	189	50.181	17.468	98.083	1.00	68.55	A
ATOM	1363	NE	ARG	189	48.754	17.670	97.855	1.00	70.63	A
ATOM	1364	CZ	ARG	189	47.906	18.095	98.784	1.00	72.05	A
ATOM	1365	NH1	ARG	189	48.340	18.362	100.010	1.00	72.50	A
ATOM	1366	NH2	ARG	189	46.623	18.252	98.484	1.00	72.44	A
ATOM	1367	C	ARG	189	50.402	13.316	95.321	1.00	63.14	A
ATOM	1368	O	ARG	189	51.085	12.537	94.652	1.00	63.21	A
ATOM	1369	N	ASN	190	49.377	12.916	96.070	1.00	64.30	A
ATOM	1370	CA	ASN	190	49.000	11.509	96.140	1.00	65.20	A
ATOM	1371	CB	ASN	190	48.225	11.220	97.439	1.00	66.56	A
ATOM	1372	CG	ASN	190	47.172	12.273	97.753	1.00	67.73	A

ATOM	1373	OD1	ASN	190	47.491	13.443	97.982	1.00	67.83	A
ATOM	1374	ND2	ASN	190	45.909	11.858	97.773	1.00	67.20	A
ATOM	1375	C	ASN	190	48.197	11.061	94.918	1.00	64.94	A
ATOM	1376	O	ASN	190	47.182	11.662	94.565	1.00	64.53	A
ATOM	1377	N	LYS	191	48.669	9.999	94.273	1.00	64.72	A
ATOM	1378	CA	LYS	191	48.018	9.463	93.083	1.00	63.98	A
ATOM	1379	CB	LYS	191	48.810	8.266	92.541	1.00	65.18	A
ATOM	1380	CG	LYS	191	48.799	7.041	93.447	1.00	66.13	A
ATOM	1381	CD	LYS	191	49.405	5.830	92.747	1.00	67.02	A
ATOM	1382	CE	LYS	191	49.274	4.572	93.593	1.00	68.29	A
ATOM	1383	NZ	LYS	191	49.860	3.375	92.919	1.00	69.29	A
ATOM	1384	C	LYS	191	46.577	9.039	93.358	1.00	62.26	A
ATOM	1385	O	LYS	191	46.151	8.963	94.513	1.00	63.17	A
ATOM	1386	N	ARG	192	45.843	8.756	92.282	1.00	58.36	A
ATOM	1387	CA	ARG	192	44.440	8.350	92.348	1.00	54.26	A
ATOM	1388	CB	ARG	192	44.308	6.833	92.578	1.00	56.88	A
ATOM	1389	CG	ARG	192	44.776	6.289	93.926	1.00	59.69	A
ATOM	1390	CD	ARG	192	43.939	5.062	94.306	1.00	62.18	A
ATOM	1391	NE	ARG	192	44.633	4.121	95.181	1.00	64.60	A
ATOM	1392	CZ	ARG	192	45.640	3.344	94.792	1.00	66.61	A
ATOM	1393	NH1	ARG	192	46.074	3.400	93.539	1.00	66.97	A
ATOM	1394	NH2	ARG	192	46.209	2.505	95.650	1.00	67.30	A
ATOM	1395	C	ARG	192	43.619	9.106	93.391	1.00	50.08	A
ATOM	1396	O	ARG	192	42.742	8.538	94.049	1.00	50.87	A
ATOM	1397	N	GLY	193	43.909	10.395	93.531	1.00	44.14	A
ATOM	1398	CA	GLY	193	43.183	11.231	94.469	1.00	35.61	A
ATOM	1399	C	GLY	193	42.799	12.482	93.712	1.00	30.34	A
ATOM	1400	O	GLY	193	43.343	12.732	92.639	1.00	30.32	A
ATOM	1401	N	VAL	194	41.865	13.264	94.238	1.00	25.49	A
ATOM	1402	CA	VAL	194	41.463	14.489	93.557	1.00	21.22	A
ATOM	1403	CB	VAL	194	40.078	14.359	92.884	1.00	20.31	A
ATOM	1404	CG1	VAL	194	40.100	13.289	91.809	1.00	19.29	A
ATOM	1405	CG2	VAL	194	39.032	14.059	93.935	1.00	18.96	A
ATOM	1406	C	VAL	194	41.375	15.668	94.505	1.00	20.08	A
ATOM	1407	O	VAL	194	41.417	15.515	95.722	1.00	20.27	A
ATOM	1408	N	ILE	195	41.238	16.853	93.930	1.00	20.12	A
ATOM	1409	CA	ILE	195	41.109	18.065	94.713	1.00	18.57	A
ATOM	1410	CB	ILE	195	42.298	19.014	94.477	1.00	20.69	A
ATOM	1411	CG2	ILE	195	42.011	20.362	95.118	1.00	21.74	A
ATOM	1412	CG1	ILE	195	43.584	18.392	95.029	1.00	21.99	A
ATOM	1413	CD1	ILE	195	44.853	19.212	94.722	1.00	23.27	A
ATOM	1414	C	ILE	195	39.838	18.791	94.297	1.00	17.41	A
ATOM	1415	O	ILE	195	39.639	19.077	93.115	1.00	15.50	A
ATOM	1416	N	ILE	196	38.962	19.066	95.256	1.00	17.01	A
ATOM	1417	CA	ILE	196	37.751	19.805	94.939	1.00	18.54	A
ATOM	1418	CB	ILE	196	36.493	19.251	95.639	1.00	18.28	A
ATOM	1419	CG2	ILE	196	35.299	20.143	95.314	1.00	13.69	A
ATOM	1420	CG1	ILE	196	36.209	17.819	95.171	1.00	17.38	A
ATOM	1421	CD1	ILE	196	37.016	16.775	95.894	1.00	21.62	A
ATOM	1422	C	ILE	196	37.981	21.232	95.407	1.00	20.22	A
ATOM	1423	O	ILE	196	38.001	21.517	96.606	1.00	20.32	A
ATOM	1424	N	LYS	197	38.158	22.122	94.441	1.00	21.72	A
ATOM	1425	CA	LYS	197	38.418	23.524	94.709	1.00	23.72	A
ATOM	1426	CB	LYS	197	38.807	24.209	93.397	1.00	26.40	A
ATOM	1427	CG	LYS	197	39.068	25.693	93.481	1.00	29.01	A
ATOM	1428	CD	LYS	197	39.519	26.211	92.125	1.00	32.62	A
ATOM	1429	CE	LYS	197	39.538	27.728	92.088	1.00	33.50	A
ATOM	1430	NZ	LYS	197	38.172	28.259	92.341	1.00	36.03	A
ATOM	1431	C	LYS	197	37.226	24.225	95.348	1.00	24.04	A
ATOM	1432	O	LYS	197	36.139	24.261	94.782	1.00	24.54	A
ATOM	1433	N	GLY	198	37.436	24.763	96.543	1.00	24.46	A
ATOM	1434	CA	GLY	198	36.377	25.478	97.227	1.00	25.68	A
ATOM	1435	C	GLY	198	35.413	24.681	98.088	1.00	26.82	A
ATOM	1436	O	GLY	198	34.482	25.256	98.652	1.00	27.32	A
ATOM	1437	N	LEU	199	35.612	23.373	98.202	1.00	27.36	A
ATOM	1438	CA	LEU	199	34.714	22.558	99.017	1.00	27.19	A
ATOM	1439	CB	LEU	199	35.008	21.068	98.819	1.00	26.21	A
ATOM	1440	CG	LEU	199	33.908	20.008	99.023	1.00	27.04	A
ATOM	1441	CD1	LEU	199	34.563	18.778	99.630	1.00	25.53	A
ATOM	1442	CD2	LEU	199	32.779	20.497	99.924	1.00	24.18	A
ATOM	1443	C	LEU	199	34.920	22.925	100.484	1.00	27.51	A
ATOM	1444	O	LEU	199	36.024	22.822	101.005	1.00	28.57	A
ATOM	1445	N	GLU	200	33.856	23.346	101.150	1.00	28.60	A

ATOM	1446	CA	GLU	200	33.950	23.721	102.553	1.00	31.25	A
ATOM	1447	CB	GLU	200	32.788	24.644	102.935	1.00	34.22	A
ATOM	1448	CG	GLU	200	32.933	26.067	102.419	1.00	39.68	A
ATOM	1449	CD	GLU	200	34.051	26.823	103.108	1.00	42.07	A
ATOM	1450	OE1	GLU	200	33.921	27.118	104.317	1.00	44.27	A
ATOM	1451	OE2	GLU	200	35.065	27.120	102.443	1.00	44.71	A
ATOM	1452	C	GLU	200	33.986	22.540	103.516	1.00	30.44	A
ATOM	1453	O	GLU	200	33.381	21.497	103.282	1.00	28.54	A
ATOM	1454	N	GLU	201	34.716	22.729	104.606	1.00	30.76	A
ATOM	1455	CA	GLU	201	34.841	21.730	105.649	1.00	29.99	A
ATOM	1456	CB	GLU	201	36.281	21.247	105.742	1.00	29.82	A
ATOM	1457	CG	GLU	201	36.755	20.516	104.511	1.00	32.15	A
ATOM	1458	CD	GLU	201	38.156	19.977	104.676	1.00	35.25	A
ATOM	1459	OE1	GLU	201	38.408	19.298	105.699	1.00	34.69	A
ATOM	1460	OE2	GLU	201	39.000	20.227	103.786	1.00	36.53	A
ATOM	1461	C	GLU	201	34.439	22.418	106.943	1.00	29.40	A
ATOM	1462	O	GLU	201	35.183	23.248	107.465	1.00	30.31	A
ATOM	1463	N	ILE	202	33.256	22.089	107.449	1.00	27.91	A
ATOM	1464	CA	ILE	202	32.765	22.694	108.679	1.00	25.94	A
ATOM	1465	CB	ILE	202	31.207	22.720	108.720	1.00	27.58	A
ATOM	1466	CG2	ILE	202	30.721	23.125	110.096	1.00	24.19	A
ATOM	1467	CG1	ILE	202	30.662	23.706	107.682	1.00	28.28	A
ATOM	1468	CD1	ILE	202	30.809	23.241	106.256	1.00	30.78	A
ATOM	1469	C	ILE	202	33.277	21.932	109.889	1.00	25.41	A
ATOM	1470	O	ILE	202	33.195	20.703	109.945	1.00	25.37	A
ATOM	1471	N	THR	203	33.811	22.667	110.856	1.00	23.88	A
ATOM	1472	CA	THR	203	34.321	22.070	112.083	1.00	22.88	A
ATOM	1473	CB	THR	203	35.397	22.981	112.742	1.00	22.77	A
ATOM	1474	OG1	THR	203	36.542	23.064	111.883	1.00	23.19	A
ATOM	1475	CG2	THR	203	35.813	22.441	114.112	1.00	19.08	A
ATOM	1476	C	THR	203	33.143	21.919	113.038	1.00	22.21	A
ATOM	1477	O	THR	203	32.385	22.867	113.242	1.00	22.47	A
ATOM	1478	N	VAL	204	32.977	20.728	113.606	1.00	21.39	A
ATOM	1479	CA	VAL	204	31.891	20.474	114.549	1.00	21.47	A
ATOM	1480	CB	VAL	204	31.248	19.102	114.278	1.00	20.28	A
ATOM	1481	CG1	VAL	204	30.034	18.906	115.162	1.00	21.96	A
ATOM	1482	CG2	VAL	204	30.859	19.000	112.820	1.00	20.66	A
ATOM	1483	C	VAL	204	32.531	20.490	115.939	1.00	23.52	A
ATOM	1484	O	VAL	204	33.083	19.484	116.385	1.00	24.43	A
ATOM	1485	N	HIS	205	32.468	21.635	116.615	1.00	23.51	A
ATOM	1486	CA	HIS	205	33.088	21.782	117.933	1.00	24.78	A
ATOM	1487	CB	HIS	205	32.979	23.238	118.407	1.00	24.16	A
ATOM	1488	CG	HIS	205	33.597	24.220	117.460	1.00	28.16	A
ATOM	1489	CD2	HIS	205	34.887	24.595	117.281	1.00	28.25	A
ATOM	1490	ND1	HIS	205	32.870	24.885	116.493	1.00	29.05	A
ATOM	1491	CE1	HIS	205	33.684	25.623	115.759	1.00	27.33	A
ATOM	1492	NE2	HIS	205	34.914	25.464	116.216	1.00	28.33	A
ATOM	1493	C	HIS	205	32.586	20.836	119.018	1.00	24.15	A
ATOM	1494	O	HIS	205	33.341	20.445	119.909	1.00	24.11	A
ATOM	1495	N	ASN	206	31.318	20.458	118.945	1.00	25.62	A
ATOM	1496	CA	ASN	206	30.758	19.552	119.939	1.00	26.43	A
ATOM	1497	CB	ASN	206	30.598	20.275	121.281	1.00	25.52	A
ATOM	1498	CG	ASN	206	29.689	21.488	121.186	1.00	26.18	A
ATOM	1499	OD1	ASN	206	28.498	21.358	120.906	1.00	28.63	A
ATOM	1500	ND2	ASN	206	30.246	22.671	121.414	1.00	24.14	A
ATOM	1501	C	ASN	206	29.422	18.960	119.496	1.00	27.20	A
ATOM	1502	O	ASN	206	28.804	19.416	118.533	1.00	27.37	A
ATOM	1503	N	LYS	207	28.993	17.933	120.212	1.00	27.93	A
ATOM	1504	CA	LYS	207	27.751	17.243	119.924	1.00	30.13	A
ATOM	1505	CB	LYS	207	27.449	16.252	121.060	1.00	32.58	A
ATOM	1506	CG	LYS	207	26.151	15.481	120.906	1.00	36.84	A
ATOM	1507	CD	LYS	207	25.112	15.921	121.929	1.00	40.39	A
ATOM	1508	CE	LYS	207	25.525	15.543	123.349	1.00	41.61	A
ATOM	1509	NZ	LYS	207	24.489	15.948	124.350	1.00	43.85	A
ATOM	1510	C	LYS	207	26.571	18.196	119.725	1.00	29.76	A
ATOM	1511	O	LYS	207	25.738	17.972	118.850	1.00	30.05	A
ATOM	1512	N	ASP	208	26.505	19.260	120.523	1.00	28.95	A
ATOM	1513	CA	ASP	208	25.402	20.214	120.429	1.00	27.71	A
ATOM	1514	CB	ASP	208	25.280	20.981	121.751	1.00	28.92	A
ATOM	1515	CG	ASP	208	24.772	20.093	122.895	1.00	33.21	A
ATOM	1516	OD1	ASP	208	24.967	20.444	124.081	1.00	32.92	A
ATOM	1517	OD2	ASP	208	24.165	19.037	122.609	1.00	34.60	A
ATOM	1518	C	ASP	208	25.524	21.169	119.240	1.00	26.33	A

ATOM	1519	O	ASP	208	24.836	22.186	119.156	1.00	26.39	A
ATOM	1520	N	GLU	209	26.381	20.810	118.296	1.00	24.27	A
ATOM	1521	CA	GLU	209	26.580	21.630	117.116	1.00	21.87	A
ATOM	1522	CB	GLU	209	28.039	22.074	117.066	1.00	23.60	A
ATOM	1523	CG	GLU	209	28.331	23.202	116.106	1.00	25.30	A
ATOM	1524	CD	GLU	209	29.678	23.849	116.384	1.00	25.66	A
ATOM	1525	OE1	GLU	209	29.872	24.362	117.507	1.00	25.63	A
ATOM	1526	OE2	GLU	209	30.538	23.845	115.481	1.00	26.97	A
ATOM	1527	C	GLU	209	26.217	20.819	115.874	1.00	19.67	A
ATOM	1528	O	GLU	209	26.125	21.350	114.769	1.00	18.53	A
ATOM	1529	N	VAL	210	25.988	19.528	116.075	1.00	16.60	A
ATOM	1530	CA	VAL	210	25.648	18.625	114.985	1.00	17.06	A
ATOM	1531	CB	VAL	210	25.654	17.148	115.479	1.00	17.27	A
ATOM	1532	CG1	VAL	210	25.307	16.224	114.330	1.00	18.17	A
ATOM	1533	CG2	VAL	210	27.028	16.779	116.068	1.00	17.55	A
ATOM	1534	C	VAL	210	24.305	18.895	114.270	1.00	16.45	A
ATOM	1535	O	VAL	210	24.267	19.119	113.063	1.00	17.67	A
ATOM	1536	N	TYR	211	23.203	18.882	115.003	1.00	14.85	A
ATOM	1537	CA	TYR	211	21.911	19.072	114.366	1.00	15.99	A
ATOM	1538	CB	TYR	211	20.789	19.050	115.404	1.00	14.76	A
ATOM	1539	CG	TYR	211	19.431	18.850	114.780	1.00	14.73	A
ATOM	1540	CD1	TYR	211	19.179	17.755	113.953	1.00	12.63	A
ATOM	1541	CE1	TYR	211	17.923	17.557	113.387	1.00	14.15	A
ATOM	1542	CD2	TYR	211	18.395	19.746	115.025	1.00	15.52	A
ATOM	1543	CE2	TYR	211	17.136	19.559	114.466	1.00	16.40	A
ATOM	1544	CZ	TYR	211	16.903	18.462	113.649	1.00	15.49	A
ATOM	1545	OH	TYR	211	15.645	18.271	113.116	1.00	12.99	A
ATOM	1546	C	TYR	211	21.763	20.303	113.483	1.00	15.43	A
ATOM	1547	O	TYR	211	21.220	20.207	112.383	1.00	17.14	A
ATOM	1548	N	GLN	212	22.238	21.456	113.925	1.00	15.05	A
ATOM	1549	CA	GLN	212	22.080	22.624	113.081	1.00	17.00	A
ATOM	1550	CB	GLN	212	22.384	23.912	113.855	1.00	18.93	A
ATOM	1551	CG	GLN	212	23.803	24.099	114.319	1.00	25.15	A
ATOM	1552	CD	GLN	212	23.892	25.178	115.379	1.00	29.02	A
ATOM	1553	OE1	GLN	212	23.354	26.276	115.209	1.00	30.43	A
ATOM	1554	NE2	GLN	212	24.562	24.870	116.486	1.00	30.19	A
ATOM	1555	C	GLN	212	22.903	22.543	111.799	1.00	16.71	A
ATOM	1556	O	GLN	212	22.459	23.030	110.749	1.00	16.05	A
ATOM	1557	N	ILE	213	24.077	21.913	111.865	1.00	14.80	A
ATOM	1558	CA	ILE	213	24.921	21.776	110.678	1.00	13.74	A
ATOM	1559	CB	ILE	213	26.309	21.148	111.036	1.00	14.83	A
ATOM	1560	CG2	ILE	213	27.118	20.846	109.764	1.00	11.99	A
ATOM	1561	CG1	ILE	213	27.099	22.122	111.926	1.00	13.49	A
ATOM	1562	CD1	ILE	213	28.495	21.607	112.366	1.00	12.70	A
ATOM	1563	C	ILE	213	24.170	20.909	109.662	1.00	14.25	A
ATOM	1564	O	ILE	213	24.135	21.223	108.474	1.00	14.16	A
ATOM	1565	N	LEU	214	23.546	19.838	110.142	1.00	12.87	A
ATOM	1566	CA	LEU	214	22.778	18.968	109.273	1.00	13.78	A
ATOM	1567	CB	LEU	214	22.355	17.705	110.022	1.00	11.53	A
ATOM	1568	CG	LEU	214	23.467	16.843	110.623	1.00	10.45	A
ATOM	1569	CD1	LEU	214	22.840	15.626	111.257	1.00	10.08	A
ATOM	1570	CD2	LEU	214	24.454	16.418	109.552	1.00	9.12	A
ATOM	1571	C	LEU	214	21.536	19.695	108.749	1.00	16.52	A
ATOM	1572	O	LEU	214	21.172	19.527	107.591	1.00	19.62	A
ATOM	1573	N	GLU	215	20.881	20.495	109.590	1.00	16.71	A
ATOM	1574	CA	GLU	215	19.690	21.239	109.152	1.00	19.78	A
ATOM	1575	CB	GLU	215	19.085	22.053	110.306	1.00	19.90	A
ATOM	1576	CG	GLU	215	18.435	21.249	111.418	1.00	21.54	A
ATOM	1577	CD	GLU	215	17.901	22.154	112.513	1.00	24.54	A
ATOM	1578	OE1	GLU	215	16.661	22.267	112.659	1.00	25.81	A
ATOM	1579	OE2	GLU	215	18.728	22.768	113.219	1.00	23.71	A
ATOM	1580	C	GLU	215	20.049	22.211	108.025	1.00	20.52	A
ATOM	1581	O	GLU	215	19.311	22.361	107.048	1.00	19.08	A
ATOM	1582	N	LYS	216	21.189	22.878	108.189	1.00	21.26	A
ATOM	1583	CA	LYS	216	21.677	23.840	107.215	1.00	22.33	A
ATOM	1584	CB	LYS	216	23.046	24.367	107.656	1.00	24.51	A
ATOM	1585	CG	LYS	216	23.510	25.619	106.938	1.00	28.98	A
ATOM	1586	CD	LYS	216	22.872	26.865	107.523	1.00	33.02	A
ATOM	1587	CE	LYS	216	23.331	27.078	108.959	1.00	35.90	A
ATOM	1588	NZ	LYS	216	24.819	27.142	109.072	1.00	37.29	A
ATOM	1589	C	LYS	216	21.782	23.150	105.850	1.00	22.36	A
ATOM	1590	O	LYS	216	21.371	23.708	104.832	1.00	23.95	A
ATOM	1591	N	GLY	217	22.318	21.931	105.838	1.00	20.62	A

ATOM	1592	CA	GLY	217	22.458	21.193	104.595	1.00	19.15	A
ATOM	1593	C	GLY	217	21.119	20.836	103.976	1.00	19.07	A
ATOM	1594	O	GLY	217	20.938	20.932	102.760	1.00	18.70	A
ATOM	1595	N	ALA	218	20.168	20.431	104.812	1.00	17.10	A
ATOM	1596	CA	ALA	218	18.845	20.070	104.330	1.00	15.84	A
ATOM	1597	CB	ALA	218	17.996	19.525	105.471	1.00	14.05	A
ATOM	1598	C	ALA	218	18.157	21.275	103.696	1.00	15.48	A
ATOM	1599	O	ALA	218	17.533	21.155	102.638	1.00	15.90	A
ATOM	1600	N	ALA	219	18.273	22.436	104.331	1.00	14.41	A
ATOM	1601	CA	ALA	219	17.638	23.642	103.800	1.00	14.13	A
ATOM	1602	CB	ALA	219	17.776	24.799	104.787	1.00	12.71	A
ATOM	1603	C	ALA	219	18.208	24.051	102.452	1.00	13.46	A
ATOM	1604	O	ALA	219	17.469	24.441	101.561	1.00	13.70	A
ATOM	1605	N	LYS	220	19.525	23.978	102.304	1.00	13.95	A
ATOM	1606	CA	LYS	220	20.146	24.357	101.045	1.00	14.23	A
ATOM	1607	CB	LYS	220	21.666	24.380	101.192	1.00	12.72	A
ATOM	1608	CG	LYS	220	22.360	25.077	100.038	1.00	17.07	A
ATOM	1609	CD	LYS	220	23.833	25.326	100.309	1.00	15.93	A
ATOM	1610	CE	LYS	220	24.512	25.923	99.080	1.00	17.58	A
ATOM	1611	NZ	LYS	220	25.991	26.097	99.261	1.00	15.01	A
ATOM	1612	C	LYS	220	19.718	23.360	99.969	1.00	14.89	A
ATOM	1613	O	LYS	220	19.497	23.722	98.809	1.00	15.14	A
ATOM	1614	N	ARG	221	19.572	22.105	100.380	1.00	14.35	A
ATOM	1615	CA	ARG	221	19.166	21.024	99.492	1.00	15.09	A
ATOM	1616	CB	ARG	221	19.185	19.714	100.274	1.00	14.48	A
ATOM	1617	CG	ARG	221	19.467	18.488	99.455	1.00	18.77	A
ATOM	1618	CD	ARG	221	19.485	17.273	100.365	1.00	20.34	A
ATOM	1619	NE	ARG	221	20.806	16.655	100.446	1.00	21.59	A
ATOM	1620	CZ	ARG	221	21.148	15.748	101.357	1.00	21.60	A
ATOM	1621	NH1	ARG	221	20.264	15.361	102.272	1.00	19.86	A
ATOM	1622	NH2	ARG	221	22.367	15.218	101.344	1.00	19.97	A
ATOM	1623	C	ARG	221	17.761	21.290	98.932	1.00	15.56	A
ATOM	1624	O	ARG	221	17.419	20.858	97.827	1.00	15.28	A
ATOM	1625	N	THR	222	16.945	22.004	99.698	1.00	14.05	A
ATOM	1626	CA	THR	222	15.608	22.325	99.253	1.00	13.31	A
ATOM	1627	CB	THR	222	14.781	22.963	100.384	1.00	16.22	A
ATOM	1628	OG1	THR	222	14.707	22.058	101.495	1.00	16.19	A
ATOM	1629	CG2	THR	222	13.367	23.252	99.904	1.00	17.44	A
ATOM	1630	C	THR	222	15.679	23.284	98.061	1.00	13.31	A
ATOM	1631	O	THR	222	14.850	23.205	97.156	1.00	12.26	A
ATOM	1632	N	THR	223	16.667	24.175	98.044	1.00	11.79	A
ATOM	1633	CA	THR	223	16.787	25.112	96.936	1.00	13.70	A
ATOM	1634	CB	THR	223	17.675	26.345	97.287	1.00	14.50	A
ATOM	1635	OG1	THR	223	19.058	25.979	97.247	1.00	18.73	A
ATOM	1636	CG2	THR	223	17.343	26.870	98.669	1.00	10.63	A
ATOM	1637	C	THR	223	17.387	24.398	95.729	1.00	15.22	A
ATOM	1638	O	THR	223	17.148	24.778	94.580	1.00	17.54	A
ATOM	1639	N	ALA	224	18.176	23.361	95.986	1.00	14.46	A
ATOM	1640	CA	ALA	224	18.773	22.607	94.896	1.00	13.62	A
ATOM	1641	CB	ALA	224	19.793	21.615	95.432	1.00	14.83	A
ATOM	1642	C	ALA	224	17.665	21.867	94.171	1.00	13.10	A
ATOM	1643	O	ALA	224	17.672	21.775	92.958	1.00	13.24	A
ATOM	1644	N	ALA	225	16.710	21.346	94.932	1.00	13.91	A
ATOM	1645	CA	ALA	225	15.598	20.596	94.369	1.00	15.07	A
ATOM	1646	CB	ALA	225	14.817	19.903	95.498	1.00	15.97	A
ATOM	1647	C	ALA	225	14.640	21.422	93.498	1.00	14.78	A
ATOM	1648	O	ALA	225	14.070	20.908	92.532	1.00	13.24	A
ATOM	1649	N	THR	226	14.449	22.694	93.822	1.00	15.56	A
ATOM	1650	CA	THR	226	13.555	23.490	92.995	1.00	16.82	A
ATOM	1651	CB	THR	226	12.992	24.729	93.747	1.00	17.66	A
ATOM	1652	OG1	THR	226	13.314	25.921	93.015	1.00	21.16	A
ATOM	1653	CG2	THR	226	13.557	24.822	95.142	1.00	16.64	A
ATOM	1654	C	THR	226	14.300	23.943	91.745	1.00	15.61	A
ATOM	1655	O	THR	226	13.685	24.257	90.726	1.00	13.81	A
ATOM	1656	N	LEU	227	15.629	23.947	91.828	1.00	14.58	A
ATOM	1657	CA	LEU	227	16.473	24.361	90.716	1.00	14.64	A
ATOM	1658	CB	LEU	227	17.751	24.993	91.267	1.00	17.19	A
ATOM	1659	CG	LEU	227	18.827	25.459	90.285	1.00	22.76	A
ATOM	1660	CD1	LEU	227	18.209	26.283	89.160	1.00	21.40	A
ATOM	1661	CD2	LEU	227	19.873	26.272	91.055	1.00	24.08	A
ATOM	1662	C	LEU	227	16.808	23.223	89.742	1.00	15.20	A
ATOM	1663	O	LEU	227	16.939	23.453	88.540	1.00	16.19	A
ATOM	1664	N	MET	228	16.924	22.000	90.256	1.00	13.63	A

ATOM	1665	CA	MET	228	17.244	20.842	89.424	1.00	14.22	A
ATOM	1666	CB	MET	228	18.607	20.275	89.852	1.00	17.08	A
ATOM	1667	CG	MET	228	19.771	21.243	89.583	1.00	18.22	A
ATOM	1668	SD	MET	228	21.340	20.816	90.414	1.00	19.64	A
ATOM	1669	CE	MET	228	21.189	21.761	91.964	1.00	16.95	A
ATOM	1670	C	MET	228	16.148	19.768	89.504	1.00	13.11	A
ATOM	1671	O	MET	228	15.683	19.423	90.588	1.00	10.34	A
ATOM	1672	N	ASN	229	15.748	19.243	88.348	1.00	12.86	A
ATOM	1673	CA	ASN	229	14.676	18.246	88.259	1.00	13.74	A
ATOM	1674	CB	ASN	229	14.319	17.975	86.794	1.00	13.77	A
ATOM	1675	CG	ASN	229	13.993	19.241	86.023	1.00	15.98	A
ATOM	1676	OD1	ASN	229	13.899	19.221	84.790	1.00	16.80	A
ATOM	1677	ND2	ASN	229	13.814	20.352	86.740	1.00	15.44	A
ATOM	1678	C	ASN	229	14.976	16.915	88.930	1.00	14.79	A
ATOM	1679	O	ASN	229	16.036	16.322	88.713	1.00	15.96	A
ATOM	1680	N	ALA	230	14.022	16.444	89.728	1.00	12.65	A
ATOM	1681	CA	ALA	230	14.155	15.182	90.443	1.00	13.20	A
ATOM	1682	CB	ALA	230	13.971	14.010	89.476	1.00	11.65	A
ATOM	1683	C	ALA	230	15.514	15.099	91.114	1.00	12.14	A
ATOM	1684	O	ALA	230	16.187	14.071	91.056	1.00	11.89	A
ATOM	1685	N	TYR	231	15.906	16.190	91.753	1.00	11.37	A
ATOM	1686	CA	TYR	231	17.190	16.270	92.435	1.00	12.67	A
ATOM	1687	CB	TYR	231	17.325	17.625	93.128	1.00	13.10	A
ATOM	1688	CG	TYR	231	18.685	17.843	93.720	1.00	13.58	A
ATOM	1689	CD1	TYR	231	18.951	17.526	95.050	1.00	15.59	A
ATOM	1690	CE1	TYR	231	20.235	17.687	95.583	1.00	15.33	A
ATOM	1691	CD2	TYR	231	19.728	18.325	92.934	1.00	14.58	A
ATOM	1692	CE2	TYR	231	21.008	18.489	93.454	1.00	15.62	A
ATOM	1693	CZ	TYR	231	21.251	18.169	94.777	1.00	14.53	A
ATOM	1694	OH	TYR	231	22.508	18.355	95.291	1.00	16.72	A
ATOM	1695	C	TYR	231	17.431	15.162	93.458	1.00	12.52	A
ATOM	1696	O	TYR	231	18.470	14.500	93.436	1.00	12.31	A
ATOM	1697	N	SER	232	16.457	14.968	94.341	1.00	12.51	A
ATOM	1698	CA	SER	232	16.543	13.978	95.406	1.00	11.76	A
ATOM	1699	CB	SER	232	15.325	14.091	96.331	1.00	10.64	A
ATOM	1700	OG	SER	232	14.143	13.654	95.692	1.00	10.59	A
ATOM	1701	C	SER	232	16.691	12.534	94.936	1.00	12.25	A
ATOM	1702	O	SER	232	17.123	11.673	95.702	1.00	12.40	A
ATOM	1703	N	SER	233	16.332	12.244	93.695	1.00	11.36	A
ATOM	1704	CA	SER	233	16.485	10.876	93.241	1.00	12.78	A
ATOM	1705	CB	SER	233	15.146	10.341	92.712	1.00	13.58	A
ATOM	1706	OG	SER	233	14.735	11.011	91.547	1.00	17.87	A
ATOM	1707	C	SER	233	17.598	10.719	92.199	1.00	12.96	A
ATOM	1708	O	SER	233	18.129	9.628	92.018	1.00	12.33	A
ATOM	1709	N	ARG	234	17.984	11.817	91.552	1.00	13.08	A
ATOM	1710	CA	ARG	234	19.022	11.770	90.519	1.00	12.98	A
ATOM	1711	CB	ARG	234	18.639	12.658	89.333	1.00	13.88	A
ATOM	1712	CG	ARG	234	17.411	12.209	88.575	1.00	15.89	A
ATOM	1713	CD	ARG	234	17.135	13.146	87.408	1.00	16.18	A
ATOM	1714	NE	ARG	234	15.961	12.713	86.672	1.00	20.62	A
ATOM	1715	CZ	ARG	234	15.330	13.442	85.761	1.00	21.81	A
ATOM	1716	NH1	ARG	234	15.764	14.662	85.459	1.00	21.30	A
ATOM	1717	NH2	ARG	234	14.249	12.951	85.168	1.00	21.53	A
ATOM	1718	C	ARG	234	20.409	12.182	90.972	1.00	11.75	A
ATOM	1719	O	ARG	234	21.374	12.011	90.230	1.00	11.05	A
ATOM	1720	N	SER	235	20.510	12.744	92.170	1.00	9.69	A
ATOM	1721	CA	SER	235	21.802	13.185	92.679	1.00	9.62	A
ATOM	1722	CB	SER	235	21.656	14.525	93.409	1.00	9.37	A
ATOM	1723	OG	SER	235	20.858	14.410	94.575	1.00	9.00	A
ATOM	1724	C	SER	235	22.445	12.171	93.617	1.00	9.66	A
ATOM	1725	O	SER	235	21.768	11.317	94.190	1.00	12.40	A
ATOM	1726	N	HIS	236	23.762	12.287	93.758	1.00	8.64	A
ATOM	1727	CA	HIS	236	24.573	11.436	94.627	1.00	5.39	A
ATOM	1728	CB	HIS	236	25.795	10.898	93.878	1.00	6.60	A
ATOM	1729	CG	HIS	236	25.474	10.085	92.666	1.00	6.36	A
ATOM	1730	CD2	HIS	236	25.516	10.398	91.350	1.00	6.40	A
ATOM	1731	ND1	HIS	236	25.109	8.758	92.732	1.00	6.26	A
ATOM	1732	CE1	HIS	236	24.945	8.287	91.509	1.00	4.95	A
ATOM	1733	NE2	HIS	236	25.186	9.261	90.652	1.00	5.93	A
ATOM	1734	C	HIS	236	25.092	12.348	95.732	1.00	6.58	A
ATOM	1735	O	HIS	236	25.676	13.396	95.446	1.00	5.89	A
ATOM	1736	N	SER	237	24.902	11.972	96.990	1.00	7.32	A
ATOM	1737	CA	SER	237	25.409	12.816	98.063	1.00	7.91	A

ATOM	1738	CB	SER	237	24.287	13.204	99.022	1.00	8.40	A
ATOM	1739	OG	SER	237	23.895	12.093	99.805	1.00	12.48	A
ATOM	1740	C	SER	237	26.505	12.089	98.830	1.00	7.51	A
ATOM	1741	O	SER	237	26.365	10.916	99.179	1.00	10.56	A
ATOM	1742	N	VAL	238	27.593	12.794	99.092	1.00	7.01	A
ATOM	1743	CA	VAL	238	28.714	12.236	99.822	1.00	7.37	A
ATOM	1744	CB	VAL	238	30.032	12.305	98.998	1.00	8.80	A
ATOM	1745	CG1	VAL	238	31.145	11.578	99.741	1.00	6.78	A
ATOM	1746	CG2	VAL	238	29.833	11.711	97.603	1.00	5.26	A
ATOM	1747	C	VAL	238	28.938	13.025	101.107	1.00	8.29	A
ATOM	1748	O	VAL	238	29.445	14.141	101.057	1.00	8.87	A
ATOM	1749	N	PHE	239	28.549	12.454	102.247	1.00	7.65	A
ATOM	1750	CA	PHE	239	28.756	13.114	103.531	1.00	7.41	A
ATOM	1751	CB	PHE	239	27.557	12.895	104.454	1.00	7.34	A
ATOM	1752	CG	PHE	239	27.615	13.694	105.726	1.00	6.91	A
ATOM	1753	CD1	PHE	239	28.508	13.355	106.744	1.00	7.70	A
ATOM	1754	CD2	PHE	239	26.778	14.788	105.906	1.00	6.68	A
ATOM	1755	CE1	PHE	239	28.567	14.102	107.931	1.00	7.54	A
ATOM	1756	CE2	PHE	239	26.828	15.546	107.086	1.00	8.52	A
ATOM	1757	CZ	PHE	239	27.724	15.201	108.101	1.00	7.57	A
ATOM	1758	C	PHE	239	30.016	12.525	104.169	1.00	10.17	A
ATOM	1759	O	PHE	239	30.063	11.334	104.486	1.00	10.87	A
ATOM	1760	N	SER	240	31.036	13.356	104.350	1.00	9.89	A
ATOM	1761	CA	SER	240	32.283	12.893	104.926	1.00	11.46	A
ATOM	1762	CB	SER	240	33.441	13.168	103.966	1.00	10.05	A
ATOM	1763	OG	SER	240	33.183	12.621	102.681	1.00	14.59	A
ATOM	1764	C	SER	240	32.598	13.508	106.285	1.00	12.92	A
ATOM	1765	O	SER	240	32.405	14.705	106.509	1.00	12.61	A
ATOM	1766	N	VAL	241	33.078	12.665	107.193	1.00	12.52	A
ATOM	1767	CA	VAL	241	33.468	13.113	108.511	1.00	13.59	A
ATOM	1768	CB	VAL	241	32.559	12.501	109.613	1.00	14.83	A
ATOM	1769	CG1	VAL	241	32.526	10.991	109.492	1.00	17.21	A
ATOM	1770	CG2	VAL	241	33.054	12.922	110.993	1.00	13.88	A
ATOM	1771	C	VAL	241	34.931	12.718	108.731	1.00	13.59	A
ATOM	1772	O	VAL	241	35.305	11.548	108.607	1.00	10.71	A
ATOM	1773	N	THR	242	35.759	13.715	109.024	1.00	14.44	A
ATOM	1774	CA	THR	242	37.175	13.489	109.264	1.00	15.80	A
ATOM	1775	CB	THR	242	38.051	14.421	108.409	1.00	16.64	A
ATOM	1776	OG1	THR	242	37.719	14.238	107.025	1.00	19.41	A
ATOM	1777	CG2	THR	242	39.539	14.102	108.618	1.00	11.48	A
ATOM	1778	C	THR	242	37.479	13.726	110.734	1.00	17.79	A
ATOM	1779	O	THR	242	37.051	14.719	111.322	1.00	19.50	A
ATOM	1780	N	ILE	243	38.224	12.805	111.326	1.00	18.66	A
ATOM	1781	CA	ILE	243	38.563	12.904	112.730	1.00	20.82	A
ATOM	1782	CB	ILE	243	37.972	11.714	113.500	1.00	20.34	A
ATOM	1783	CG2	ILE	243	38.085	11.953	114.993	1.00	20.79	A
ATOM	1784	CG1	ILE	243	36.506	11.524	113.114	1.00	21.41	A
ATOM	1785	CD1	ILE	243	35.902	10.213	113.632	1.00	20.85	A
ATOM	1786	C	ILE	243	40.076	12.928	112.958	1.00	23.56	A
ATOM	1787	O	ILE	243	40.782	11.953	112.664	1.00	23.06	A
ATOM	1788	N	HIS	244	40.574	14.053	113.458	1.00	25.26	A
ATOM	1789	CA	HIS	244	41.994	14.177	113.765	1.00	27.63	A
ATOM	1790	CB	HIS	244	42.507	15.589	113.485	1.00	28.72	A
ATOM	1791	CG	HIS	244	42.974	15.799	112.079	1.00	32.69	A
ATOM	1792	CD2	HIS	244	44.219	15.803	111.544	1.00	33.88	A
ATOM	1793	ND1	HIS	244	42.111	16.067	111.038	1.00	34.05	A
ATOM	1794	CE1	HIS	244	42.803	16.231	109.924	1.00	33.87	A
ATOM	1795	NE2	HIS	244	44.085	16.075	110.203	1.00	35.45	A
ATOM	1796	C	HIS	244	42.108	13.878	115.254	1.00	29.05	A
ATOM	1797	O	HIS	244	41.541	14.599	116.084	1.00	28.16	A
ATOM	1798	N	MET	245	42.827	12.813	115.592	1.00	29.99	A
ATOM	1799	CA	MET	245	42.968	12.425	116.988	1.00	32.41	A
ATOM	1800	CB	MET	245	42.330	11.053	117.210	1.00	30.98	A
ATOM	1801	CG	MET	245	40.880	10.959	116.795	1.00	29.47	A
ATOM	1802	SD	MET	245	40.390	9.243	116.608	1.00	28.28	A
ATOM	1803	CE	MET	245	41.018	8.925	114.953	1.00	26.37	A
ATOM	1804	C	MET	245	44.395	12.388	117.520	1.00	34.03	A
ATOM	1805	O	MET	245	45.332	11.978	116.831	1.00	33.45	A
ATOM	1806	N	LYS	246	44.536	12.821	118.765	1.00	36.79	A
ATOM	1807	CA	LYS	246	45.813	12.813	119.456	1.00	41.41	A
ATOM	1808	CB	LYS	246	46.345	14.234	119.645	1.00	44.53	A
ATOM	1809	CG	LYS	246	47.765	14.284	120.187	1.00	48.98	A
ATOM	1810	CD	LYS	246	48.360	15.678	120.048	1.00	52.77	A

ATOM	1811	CE	LYS	246	49.830	15.693	120.448	1.00	55.09	A
ATOM	1812	NZ	LYS	246	50.445	17.035	120.232	1.00	56.33	A
ATOM	1813	C	LYS	246	45.496	12.179	120.799	1.00	42.14	A
ATOM	1814	O	LYS	246	45.157	12.860	121.764	1.00	42.94	A
ATOM	1815	N	GLU	247	45.586	10.859	120.834	1.00	42.88	A
ATOM	1816	CA	GLU	247	45.286	10.090	122.027	1.00	45.27	A
ATOM	1817	CB	GLU	247	44.896	8.669	121.623	1.00	45.22	A
ATOM	1818	CG	GLU	247	44.301	7.829	122.726	1.00	45.70	A
ATOM	1819	CD	GLU	247	44.075	6.396	122.282	1.00	47.91	A
ATOM	1820	OE1	GLU	247	43.507	6.194	121.186	1.00	48.39	A
ATOM	1821	OE2	GLU	247	44.462	5.471	123.032	1.00	47.23	A
ATOM	1822	C	GLU	247	46.463	10.040	122.995	1.00	46.56	A
ATOM	1823	O	GLU	247	47.625	10.055	122.592	1.00	46.38	A
ATOM	1824	N	THR	248	46.144	9.988	124.281	1.00	47.43	A
ATOM	1825	CA	THR	248	47.155	9.903	125.320	1.00	49.03	A
ATOM	1826	CB	THR	248	47.340	11.259	126.029	1.00	49.86	A
ATOM	1827	OG1	THR	248	47.733	12.245	125.066	1.00	50.38	A
ATOM	1828	CG2	THR	248	48.416	11.162	127.104	1.00	49.64	A
ATOM	1829	C	THR	248	46.679	8.838	126.309	1.00	49.49	A
ATOM	1830	O	THR	248	45.810	9.087	127.148	1.00	49.04	A
ATOM	1831	N	THR	249	47.244	7.641	126.177	1.00	50.47	A
ATOM	1832	CA	THR	249	46.892	6.510	127.025	1.00	51.50	A
ATOM	1833	CB	THR	249	47.684	5.252	126.621	1.00	51.30	A
ATOM	1834	OG1	THR	249	49.072	5.435	126.933	1.00	50.45	A
ATOM	1835	CG2	THR	249	47.539	4.994	125.127	1.00	50.34	A
ATOM	1836	C	THR	249	47.157	6.813	128.493	1.00	52.76	A
ATOM	1837	O	THR	249	47.801	7.811	128.819	1.00	52.66	A
ATOM	1838	N	ILE	250	46.663	5.948	129.375	1.00	53.97	A
ATOM	1839	CA	ILE	250	46.842	6.136	130.812	1.00	55.19	A
ATOM	1840	CB	ILE	250	46.042	5.078	131.624	1.00	55.38	A
ATOM	1841	CG2	ILE	250	44.596	5.061	131.147	1.00	55.55	A
ATOM	1842	CG1	ILE	250	46.656	3.683	131.466	1.00	55.59	A
ATOM	1843	CD1	ILE	250	46.516	3.078	130.073	1.00	56.12	A
ATOM	1844	C	ILE	250	48.313	6.097	131.239	1.00	55.82	A
ATOM	1845	O	ILE	250	48.634	6.316	132.408	1.00	55.54	A
ATOM	1846	N	ASP	251	49.198	5.833	130.281	1.00	56.61	A
ATOM	1847	CA	ASP	251	50.633	5.776	130.543	1.00	57.44	A
ATOM	1848	CB	ASP	251	51.285	4.696	129.679	1.00	57.92	A
ATOM	1849	CG	ASP	251	50.757	3.306	129.979	1.00	58.92	A
ATOM	1850	OD1	ASP	251	50.894	2.427	129.098	1.00	59.53	A
ATOM	1851	OD2	ASP	251	50.217	3.088	131.089	1.00	57.67	A
ATOM	1852	C	ASP	251	51.271	7.124	130.222	1.00	57.89	A
ATOM	1853	O	ASP	251	51.858	7.770	131.090	1.00	59.32	A
ATOM	1854	N	GLY	252	51.141	7.537	128.967	1.00	57.36	A
ATOM	1855	CA	GLY	252	51.707	8.797	128.526	1.00	57.52	A
ATOM	1856	C	GLY	252	52.089	8.717	127.060	1.00	57.92	A
ATOM	1857	O	GLY	252	52.814	9.571	126.545	1.00	58.43	A
ATOM	1858	N	GLU	253	51.602	7.675	126.392	1.00	57.56	A
ATOM	1859	CA	GLU	253	51.869	7.456	124.974	1.00	57.81	A
ATOM	1860	CB	GLU	253	51.552	6.006	124.598	1.00	59.90	A
ATOM	1861	CG	GLU	253	52.084	4.968	125.573	1.00	62.49	A
ATOM	1862	CD	GLU	253	51.543	3.581	125.294	1.00	63.65	A
ATOM	1863	OE1	GLU	253	51.693	3.108	124.146	1.00	65.45	A
ATOM	1864	OE2	GLU	253	50.970	2.967	126.219	1.00	63.15	A
ATOM	1865	C	GLU	253	50.959	8.381	124.179	1.00	56.36	A
ATOM	1866	O	GLU	253	49.818	8.618	124.572	1.00	56.13	A
ATOM	1867	N	GLU	254	51.451	8.908	123.067	1.00	54.64	A
ATOM	1868	CA	GLU	254	50.626	9.790	122.256	1.00	53.82	A
ATOM	1869	CB	GLU	254	51.269	11.183	122.151	1.00	54.89	A
ATOM	1870	CG	GLU	254	52.568	11.259	121.354	1.00	56.86	A
ATOM	1871	CD	GLU	254	52.363	11.790	119.939	1.00	58.42	A
ATOM	1872	OE1	GLU	254	51.856	12.924	119.800	1.00	58.67	A
ATOM	1873	OE2	GLU	254	52.713	11.078	118.968	1.00	57.93	A
ATOM	1874	C	GLU	254	50.397	9.186	120.876	1.00	52.35	A
ATOM	1875	O	GLU	254	51.340	8.945	120.124	1.00	52.94	A
ATOM	1876	N	LEU	255	49.135	8.916	120.560	1.00	50.68	A
ATOM	1877	CA	LEU	255	48.772	8.340	119.268	1.00	48.63	A
ATOM	1878	CB	LEU	255	47.828	7.142	119.439	1.00	49.85	A
ATOM	1879	CG	LEU	255	48.236	5.895	120.231	1.00	52.23	A
ATOM	1880	CD1	LEU	255	49.595	5.409	119.752	1.00	53.67	A
ATOM	1881	CD2	LEU	255	48.278	6.201	121.720	1.00	53.72	A
ATOM	1882	C	LEU	255	48.069	9.381	118.413	1.00	46.05	A
ATOM	1883	O	LEU	255	46.978	9.832	118.755	1.00	45.38	A

ATOM	1884	N	VAL	256	48.695	9.772	117.310	1.00	43.74	A
ATOM	1885	CA	VAL	256	48.081	10.740	116.409	1.00	41.19	A
ATOM	1886	CB	VAL	256	49.084	11.791	115.943	1.00	40.17	A
ATOM	1887	CG1	VAL	256	48.442	12.680	114.897	1.00	38.91	A
ATOM	1888	CG2	VAL	256	49.543	12.614	117.132	1.00	40.08	A
ATOM	1889	C	VAL	256	47.533	9.994	115.200	1.00	39.59	A
ATOM	1890	O	VAL	256	48.276	9.619	114.291	1.00	39.95	A
ATOM	1891	N	LYS	257	46.221	9.780	115.212	1.00	36.47	A
ATOM	1892	CA	LYS	257	45.534	9.056	114.150	1.00	32.43	A
ATOM	1893	CB	LYS	257	44.733	7.902	114.756	1.00	31.46	A
ATOM	1894	CG	LYS	257	45.525	7.024	115.710	1.00	31.17	A
ATOM	1895	CD	LYS	257	44.613	6.174	116.573	1.00	30.49	A
ATOM	1896	CE	LYS	257	43.767	7.045	117.486	1.00	31.11	A
ATOM	1897	NZ	LYS	257	42.941	6.216	118.411	1.00	32.10	A
ATOM	1898	C	LYS	257	44.585	9.965	113.384	1.00	30.18	A
ATOM	1899	O	LYS	257	44.067	10.944	113.928	1.00	28.57	A
ATOM	1900	N	ILE	258	44.361	9.624	112.120	1.00	28.11	A
ATOM	1901	CA	ILE	258	43.451	10.372	111.263	1.00	26.14	A
ATOM	1902	CB	ILE	258	44.223	11.174	110.209	1.00	26.23	A
ATOM	1903	CG2	ILE	258	43.265	11.782	109.205	1.00	26.22	A
ATOM	1904	CG1	ILE	258	45.027	12.271	110.904	1.00	27.27	A
ATOM	1905	CD1	ILE	258	45.828	13.155	109.943	1.00	29.18	A
ATOM	1906	C	ILE	258	42.493	9.400	110.573	1.00	24.09	A
ATOM	1907	O	ILE	258	42.912	8.562	109.772	1.00	24.80	A
ATOM	1908	N	GLY	259	41.208	9.509	110.899	1.00	20.82	A
ATOM	1909	CA	GLY	259	40.221	8.629	110.300	1.00	17.04	A
ATOM	1910	C	GLY	259	39.214	9.376	109.447	1.00	15.18	A
ATOM	1911	O	GLY	259	38.843	10.502	109.765	1.00	14.10	A
ATOM	1912	N	LYS	260	38.782	8.764	108.349	1.00	13.62	A
ATOM	1913	CA	LYS	260	37.803	9.399	107.487	1.00	13.15	A
ATOM	1914	CB	LYS	260	38.480	9.983	106.247	1.00	13.95	A
ATOM	1915	CG	LYS	260	37.557	10.866	105.414	1.00	14.12	A
ATOM	1916	CD	LYS	260	38.254	11.500	104.220	1.00	14.32	A
ATOM	1917	CE	LYS	260	37.256	12.328	103.410	1.00	16.28	A
ATOM	1918	NZ	LYS	260	37.881	13.104	102.307	1.00	14.26	A
ATOM	1919	C	LYS	260	36.687	8.427	107.080	1.00	13.76	A
ATOM	1920	O	LYS	260	36.939	7.312	106.612	1.00	14.46	A
ATOM	1921	N	LEU	261	35.449	8.868	107.277	1.00	11.00	A
ATOM	1922	CA	LEU	261	34.281	8.067	106.954	1.00	9.03	A
ATOM	1923	CB	LEU	261	33.461	7.830	108.217	1.00	6.67	A
ATOM	1924	CG	LEU	261	32.123	7.109	108.093	1.00	3.68	A
ATOM	1925	CD1	LEU	261	32.319	5.722	107.514	1.00	2.23	A
ATOM	1926	CD2	LEU	261	31.499	7.027	109.470	1.00	3.51	A
ATOM	1927	C	LEU	261	33.416	8.768	105.905	1.00	10.81	A
ATOM	1928	O	LEU	261	32.978	9.914	106.113	1.00	9.03	A
ATOM	1929	N	ASN	262	33.180	8.079	104.786	1.00	8.62	A
ATOM	1930	CA	ASN	262	32.360	8.608	103.702	1.00	9.89	A
ATOM	1931	CB	ASN	262	33.042	8.371	102.348	1.00	10.45	A
ATOM	1932	CG	ASN	262	34.436	8.948	102.294	1.00	14.30	A
ATOM	1933	OD1	ASN	262	35.420	8.220	102.136	1.00	16.96	A
ATOM	1934	ND2	ASN	262	34.535	10.263	102.432	1.00	9.79	A
ATOM	1935	C	ASN	262	31.003	7.905	103.721	1.00	9.32	A
ATOM	1936	O	ASN	262	30.940	6.687	103.638	1.00	10.83	A
ATOM	1937	N	LEU	263	29.923	8.673	103.839	1.00	8.87	A
ATOM	1938	CA	LEU	263	28.572	8.108	103.874	1.00	8.66	A
ATOM	1939	CB	LEU	263	27.832	8.607	105.108	1.00	6.12	A
ATOM	1940	CG	LEU	263	28.620	8.253	106.375	1.00	8.11	A
ATOM	1941	CD1	LEU	263	27.981	8.906	107.599	1.00	8.26	A
ATOM	1942	CD2	LEU	263	28.679	6.728	106.520	1.00	5.47	A
ATOM	1943	C	LEU	263	27.878	8.545	102.595	1.00	10.21	A
ATOM	1944	O	LEU	263	27.488	9.706	102.441	1.00	12.04	A
ATOM	1945	N	VAL	264	27.716	7.597	101.682	1.00	9.38	A
ATOM	1946	CA	VAL	264	27.161	7.891	100.378	1.00	9.77	A
ATOM	1947	CB	VAL	264	28.089	7.329	99.291	1.00	10.33	A
ATOM	1948	CG1	VAL	264	27.734	7.907	97.928	1.00	8.01	A
ATOM	1949	CG2	VAL	264	29.522	7.637	99.672	1.00	8.80	A
ATOM	1950	C	VAL	264	25.765	7.403	100.104	1.00	10.32	A
ATOM	1951	O	VAL	264	25.465	6.212	100.226	1.00	12.03	A
ATOM	1952	N	ASP	265	24.925	8.355	99.714	1.00	9.00	A
ATOM	1953	CA	ASP	265	23.534	8.116	99.368	1.00	6.24	A
ATOM	1954	CB	ASP	265	22.650	9.211	99.985	1.00	5.48	A
ATOM	1955	CG	ASP	265	21.171	8.994	99.713	1.00	7.76	A
ATOM	1956	OD1	ASP	265	20.851	8.232	98.782	1.00	5.27	A

ATOM	1957	OD2	ASP	265	20.328	9.589	100.421	1.00	9.82	A
ATOM	1958	C	ASP	265	23.497	8.203	97.838	1.00	4.32	A
ATOM	1959	O	ASP	265	23.410	9.289	97.270	1.00	4.24	A
ATOM	1960	N	LEU	266	23.575	7.060	97.172	1.00	4.44	A
ATOM	1961	CA	LEU	266	23.569	7.024	95.710	1.00	5.61	A
ATOM	1962	CB	LEU	266	23.941	5.616	95.222	1.00	1.02	A
ATOM	1963	CG	LEU	266	25.345	5.124	95.622	1.00	5.57	A
ATOM	1964	CD1	LEU	266	25.561	3.649	95.242	1.00	1.02	A
ATOM	1965	CD2	LEU	266	26.379	6.020	94.942	1.00	4.62	A
ATOM	1966	C	LEU	266	22.252	7.451	95.065	1.00	7.56	A
ATOM	1967	O	LEU	266	21.190	7.438	95.694	1.00	9.23	A
ATOM	1968	N	ALA	267	22.336	7.845	93.801	1.00	7.43	A
ATOM	1969	CA	ALA	267	21.156	8.220	93.047	1.00	6.36	A
ATOM	1970	CB	ALA	267	21.572	8.756	91.687	1.00	5.05	A
ATOM	1971	C	ALA	267	20.324	6.945	92.877	1.00	6.99	A
ATOM	1972	O	ALA	267	20.844	5.840	93.020	1.00	5.27	A
ATOM	1973	N	GLY	268	19.042	7.105	92.571	1.00	9.81	A
ATOM	1974	CA	GLY	268	18.170	5.961	92.378	1.00	12.51	A
ATOM	1975	C	GLY	268	18.633	5.079	91.233	1.00	15.67	A
ATOM	1976	O	GLY	268	18.859	5.555	90.113	1.00	17.12	A
ATOM	1977	N	SER	269	18.755	3.786	91.516	1.00	15.31	A
ATOM	1978	CA	SER	269	19.220	2.802	90.543	1.00	18.23	A
ATOM	1979	CB	SER	269	19.677	1.554	91.293	1.00	17.50	A
ATOM	1980	OG	SER	269	18.596	1.027	92.043	1.00	12.64	A
ATOM	1981	C	SER	269	18.195	2.383	89.484	1.00	20.29	A
ATOM	1982	O	SER	269	18.497	1.549	88.627	1.00	19.97	A
ATOM	1983	N	GLU	270	16.994	2.950	89.537	1.00	22.91	A
ATOM	1984	CA	GLU	270	15.949	2.576	88.587	1.00	26.68	A
ATOM	1985	CB	GLU	270	14.563	2.958	89.136	1.00	24.65	A
ATOM	1986	CG	GLU	270	14.251	4.460	89.210	1.00	22.35	A
ATOM	1987	CD	GLU	270	14.960	5.185	90.349	1.00	21.47	A
ATOM	1988	OE1	GLU	270	15.545	4.524	91.234	1.00	18.55	A
ATOM	1989	OE2	GLU	270	14.922	6.433	90.354	1.00	22.04	A
ATOM	1990	C	GLU	270	16.117	3.139	87.177	1.00	31.14	A
ATOM	1991	O	GLU	270	16.608	4.256	86.981	1.00	30.32	A
ATOM	1992	N	ASN	271	15.717	2.336	86.194	1.00	36.67	A
ATOM	1993	CA	ASN	271	15.799	2.730	84.793	1.00	41.70	A
ATOM	1994	CB	ASN	271	16.856	1.900	84.059	1.00	45.31	A
ATOM	1995	CG	ASN	271	17.121	2.409	82.649	1.00	49.20	A
ATOM	1996	OD1	ASN	271	17.661	3.504	82.460	1.00	50.16	A
ATOM	1997	ND2	ASN	271	16.733	1.618	81.650	1.00	50.41	A
ATOM	1998	C	ASN	271	14.440	2.537	84.120	1.00	42.80	A
ATOM	1999	O	ASN	271	13.799	1.494	84.276	1.00	44.21	A
ATOM	2000	N	ASN	287	17.192	11.408	81.710	1.00	47.26	A
ATOM	2001	CA	ASN	287	18.348	11.168	80.854	1.00	46.49	A
ATOM	2002	CB	ASN	287	19.078	12.487	80.582	1.00	48.42	A
ATOM	2003	CG	ASN	287	18.323	13.385	79.614	1.00	51.20	A
ATOM	2004	OD1	ASN	287	18.724	14.526	79.368	1.00	51.62	A
ATOM	2005	ND2	ASN	287	17.230	12.870	79.053	1.00	50.69	A
ATOM	2006	C	ASN	287	19.324	10.139	81.437	1.00	45.61	A
ATOM	2007	O	ASN	287	18.912	9.131	82.021	1.00	45.57	A
ATOM	2008	N	ILE	288	20.619	10.400	81.285	1.00	42.07	A
ATOM	2009	CA	ILE	288	21.634	9.471	81.771	1.00	37.70	A
ATOM	2010	CB	ILE	288	22.657	9.156	80.646	1.00	39.37	A
ATOM	2011	CG2	ILE	288	21.964	8.416	79.511	1.00	38.36	A
ATOM	2012	CG1	ILE	288	23.269	10.450	80.095	1.00	40.59	A
ATOM	2013	CD1	ILE	288	24.498	10.959	80.863	1.00	42.56	A
ATOM	2014	C	ILE	288	22.385	9.924	83.019	1.00	33.61	A
ATOM	2015	O	ILE	288	22.668	11.113	83.194	1.00	34.30	A
ATOM	2016	N	ASN	289	22.682	8.970	83.897	1.00	26.00	A
ATOM	2017	CA	ASN	289	23.431	9.267	85.107	1.00	19.08	A
ATOM	2018	CB	ASN	289	22.810	8.599	86.334	1.00	17.79	A
ATOM	2019	CG	ASN	289	23.253	9.253	87.645	1.00	18.18	A
ATOM	2020	OD1	ASN	289	22.461	9.928	88.299	1.00	18.30	A
ATOM	2021	ND2	ASN	289	24.516	9.065	88.023	1.00	13.15	A
ATOM	2022	C	ASN	289	24.808	8.679	84.861	1.00	15.55	A
ATOM	2023	O	ASN	289	25.033	7.493	85.072	1.00	12.50	A
ATOM	2024	N	GLN	290	25.727	9.515	84.398	1.00	13.86	A
ATOM	2025	CA	GLN	290	27.079	9.070	84.088	1.00	12.24	A
ATOM	2026	CB	GLN	290	27.896	10.253	83.560	1.00	11.18	A
ATOM	2027	CG	GLN	290	29.284	9.913	83.068	1.00	10.23	A
ATOM	2028	CD	GLN	290	29.297	8.795	82.036	1.00	11.80	A
ATOM	2029	OE1	GLN	290	28.336	8.609	81.273	1.00	12.41	A

ATOM	2030	NE2	GLN	290	30.399	8.059	81.990	1.00	10.69	A
ATOM	2031	C	GLN	290	27.778	8.414	85.276	1.00	11.63	A
ATOM	2032	O	GLN	290	28.394	7.359	85.130	1.00	12.20	A
ATOM	2033	N	SER	291	27.662	9.023	86.452	1.00	10.76	A
ATOM	2034	CA	SER	291	28.304	8.485	87.650	1.00	11.04	A
ATOM	2035	CB	SER	291	28.163	9.450	88.830	1.00	10.12	A
ATOM	2036	OG	SER	291	29.068	10.536	88.711	1.00	11.06	A
ATOM	2037	C	SER	291	27.753	7.131	88.043	1.00	11.79	A
ATOM	2038	O	SER	291	28.512	6.241	88.420	1.00	14.45	A
ATOM	2039	N	LEU	292	26.437	6.971	87.959	1.00	11.86	A
ATOM	2040	CA	LEU	292	25.805	5.709	88.312	1.00	10.53	A
ATOM	2041	CB	LEU	292	24.278	5.875	88.329	1.00	10.11	A
ATOM	2042	CG	LEU	292	23.467	4.734	88.952	1.00	11.58	A
ATOM	2043	CD1	LEU	292	23.811	4.605	90.427	1.00	9.76	A
ATOM	2044	CD2	LEU	292	21.974	5.007	88.791	1.00	11.92	A
ATOM	2045	C	LEU	292	26.216	4.653	87.289	1.00	10.87	A
ATOM	2046	O	LEU	292	26.559	3.525	87.634	1.00	12.05	A
ATOM	2047	N	LEU	293	26.196	5.043	86.022	1.00	11.04	A
ATOM	2048	CA	LEU	293	26.566	4.165	84.929	1.00	11.19	A
ATOM	2049	CB	LEU	293	26.382	4.922	83.608	1.00	11.77	A
ATOM	2050	CG	LEU	293	25.394	4.442	82.532	1.00	15.36	A
ATOM	2051	CD1	LEU	293	24.197	3.755	83.162	1.00	13.37	A
ATOM	2052	CD2	LEU	293	24.948	5.638	81.690	1.00	11.70	A
ATOM	2053	C	LEU	293	28.026	3.714	85.094	1.00	13.10	A
ATOM	2054	O	LEU	293	28.355	2.535	84.918	1.00	13.28	A
ATOM	2055	N	THR	294	28.896	4.660	85.437	1.00	11.21	A
ATOM	2056	CA	THR	294	30.313	4.372	85.613	1.00	10.86	A
ATOM	2057	CB	THR	294	31.119	5.690	85.778	1.00	12.02	A
ATOM	2058	OG1	THR	294	30.934	6.497	84.611	1.00	11.95	A
ATOM	2059	CG2	THR	294	32.605	5.409	85.947	1.00	8.75	A
ATOM	2060	C	THR	294	30.571	3.459	86.809	1.00	11.13	A
ATOM	2061	O	THR	294	31.416	2.563	86.735	1.00	10.49	A
ATOM	2062	N	LEU	295	29.843	3.686	87.906	1.00	11.70	A
ATOM	2063	CA	LEU	295	29.983	2.870	89.117	1.00	11.27	A
ATOM	2064	CB	LEU	295	29.033	3.348	90.224	1.00	10.76	A
ATOM	2065	CG	LEU	295	28.993	2.535	91.529	1.00	10.99	A
ATOM	2066	CD1	LEU	295	30.352	2.540	92.214	1.00	12.41	A
ATOM	2067	CD2	LEU	295	27.950	3.126	92.458	1.00	10.86	A
ATOM	2068	C	LEU	295	29.683	1.424	88.788	1.00	10.80	A
ATOM	2069	O	LEU	295	30.365	0.521	89.252	1.00	12.59	A
ATOM	2070	N	GLY	296	28.652	1.205	87.986	1.00	11.95	A
ATOM	2071	CA	GLY	296	28.311	-0.153	87.607	1.00	12.43	A
ATOM	2072	C	GLY	296	29.444	-0.772	86.810	1.00	13.06	A
ATOM	2073	O	GLY	296	29.796	-1.938	87.007	1.00	15.18	A
ATOM	2074	N	ARG	297	30.021	0.014	85.906	1.00	11.06	A
ATOM	2075	CA	ARG	297	31.121	-0.458	85.086	1.00	9.97	A
ATOM	2076	CB	ARG	297	31.369	0.517	83.943	1.00	9.77	A
ATOM	2077	CG	ARG	297	30.264	0.487	82.909	1.00	10.57	A
ATOM	2078	CD	ARG	297	30.173	1.789	82.136	1.00	8.79	A
ATOM	2079	NE	ARG	297	29.014	1.776	81.259	1.00	10.33	A
ATOM	2080	CZ	ARG	297	28.492	2.853	80.685	1.00	9.93	A
ATOM	2081	NH1	ARG	297	29.033	4.044	80.892	1.00	10.65	A
ATOM	2082	NH2	ARG	297	27.412	2.740	79.920	1.00	7.47	A
ATOM	2083	C	ARG	297	32.395	-0.675	85.889	1.00	9.24	A
ATOM	2084	O	ARG	297	33.154	-1.597	85.594	1.00	10.04	A
ATOM	2085	N	VAL	298	32.632	0.164	86.897	1.00	6.73	A
ATOM	2086	CA	VAL	298	33.823	0.009	87.734	1.00	7.78	A
ATOM	2087	CB	VAL	298	33.988	1.196	88.719	1.00	7.07	A
ATOM	2088	CG1	VAL	298	35.026	0.865	89.773	1.00	2.16	A
ATOM	2089	CG2	VAL	298	34.408	2.449	87.957	1.00	4.22	A
ATOM	2090	C	VAL	298	33.775	-1.315	88.517	1.00	9.86	A
ATOM	2091	O	VAL	298	34.761	-2.057	88.556	1.00	11.69	A
ATOM	2092	N	ILE	299	32.625	-1.616	89.120	1.00	10.47	A
ATOM	2093	CA	ILE	299	32.437	-2.858	89.879	1.00	10.02	A
ATOM	2094	CB	ILE	299	31.004	-2.910	90.488	1.00	10.33	A
ATOM	2095	CG2	ILE	299	30.710	-4.280	91.095	1.00	9.07	A
ATOM	2096	CG1	ILE	299	30.869	-1.821	91.558	1.00	10.35	A
ATOM	2097	CD1	ILE	299	29.445	-1.587	92.019	1.00	13.51	A
ATOM	2098	C	ILE	299	32.659	-4.070	88.972	1.00	11.19	A
ATOM	2099	O	ILE	299	33.341	-5.019	89.348	1.00	9.09	A
ATOM	2100	N	THR	300	32.084	-4.031	87.771	1.00	14.08	A
ATOM	2101	CA	THR	300	32.227	-5.125	86.808	1.00	13.98	A
ATOM	2102	CB	THR	300	31.470	-4.813	85.506	1.00	13.76	A

ATOM	2103	OG1	THR	300	30.062	-4.803	85.770	1.00	14.55	A
ATOM	2104	CG2	THR	300	31.783	-5.848	84.436	1.00	10.43	A
ATOM	2105	C	THR	300	33.699	-5.394	86.472	1.00	16.17	A
ATOM	2106	O	THR	300	34.151	-6.536	86.533	1.00	16.23	A
ATOM	2107	N	ALA	301	34.442	-4.345	86.120	1.00	15.12	A
ATOM	2108	CA	ALA	301	35.850	-4.502	85.791	1.00	14.70	A
ATOM	2109	CB	ALA	301	36.449	-3.157	85.362	1.00	13.94	A
ATOM	2110	C	ALA	301	36.622	-5.068	86.985	1.00	14.94	A
ATOM	2111	O	ALA	301	37.512	-5.893	86.819	1.00	15.20	A
ATOM	2112	N	LEU	302	36.282	-4.620	88.188	1.00	16.14	A
ATOM	2113	CA	LEU	302	36.951	-5.101	89.392	1.00	19.53	A
ATOM	2114	CB	LEU	302	36.585	-4.222	90.594	1.00	19.74	A
ATOM	2115	CG	LEU	302	37.221	-2.830	90.688	1.00	17.91	A
ATOM	2116	CD1	LEU	302	36.558	-2.045	91.802	1.00	17.40	A
ATOM	2117	CD2	LEU	302	38.717	-2.963	90.948	1.00	15.50	A
ATOM	2118	C	LEU	302	36.643	-6.564	89.717	1.00	21.83	A
ATOM	2119	O	LEU	302	37.533	-7.302	90.127	1.00	23.13	A
ATOM	2120	N	VAL	303	35.398	-6.993	89.535	1.00	24.49	A
ATOM	2121	CA	VAL	303	35.059	-8.379	89.838	1.00	27.38	A
ATOM	2122	CB	VAL	303	33.547	-8.571	90.069	1.00	26.90	A
ATOM	2123	CG1	VAL	303	33.052	-7.570	91.101	1.00	26.40	A
ATOM	2124	CG2	VAL	303	32.796	-8.428	88.770	1.00	29.98	A
ATOM	2125	C	VAL	303	35.512	-9.341	88.744	1.00	30.52	A
ATOM	2126	O	VAL	303	35.877	-10.477	89.035	1.00	31.69	A
ATOM	2127	N	GLU	304	35.491	-8.897	87.490	1.00	32.89	A
ATOM	2128	CA	GLU	304	35.921	-9.750	86.389	1.00	35.74	A
ATOM	2129	CB	GLU	304	35.203	-9.374	85.094	1.00	37.37	A
ATOM	2130	CG	GLU	304	33.689	-9.307	85.221	1.00	39.61	A
ATOM	2131	CD	GLU	304	32.999	-9.146	83.876	1.00	42.09	A
ATOM	2132	OE1	GLU	304	33.515	-8.380	83.028	1.00	42.71	A
ATOM	2133	OE2	GLU	304	31.939	-9.775	83.671	1.00	41.78	A
ATOM	2134	C	GLU	304	37.426	-9.604	86.206	1.00	37.86	A
ATOM	2135	O	GLU	304	37.996	-10.078	85.227	1.00	37.10	A
ATOM	2136	N	ARG	305	38.054	-8.937	87.169	1.00	40.46	A
ATOM	2137	CA	ARG	305	39.496	-8.716	87.177	1.00	42.89	A
ATOM	2138	CB	ARG	305	40.215	-10.025	87.534	1.00	45.84	A
ATOM	2139	CG	ARG	305	40.201	-10.328	89.040	1.00	50.55	A
ATOM	2140	CD	ARG	305	40.942	-9.222	89.795	1.00	55.95	A
ATOM	2141	NE	ARG	305	40.641	-9.139	91.227	1.00	60.56	A
ATOM	2142	CZ	ARG	305	41.079	-9.988	92.154	1.00	62.46	A
ATOM	2143	NH1	ARG	305	41.848	-11.016	91.816	1.00	63.45	A
ATOM	2144	NH2	ARG	305	40.765	-9.793	93.431	1.00	62.35	A
ATOM	2145	C	ARG	305	40.094	-8.101	85.913	1.00	43.03	A
ATOM	2146	O	ARG	305	41.257	-8.337	85.585	1.00	42.44	A
ATOM	2147	N	THR	306	39.292	-7.300	85.218	1.00	43.37	A
ATOM	2148	CA	THR	306	39.728	-6.607	84.009	1.00	43.89	A
ATOM	2149	CB	THR	306	38.553	-5.823	83.373	1.00	44.73	A
ATOM	2150	OG1	THR	306	37.525	-6.738	82.967	1.00	46.53	A
ATOM	2151	CG2	THR	306	39.021	-5.031	82.173	1.00	44.99	A
ATOM	2152	C	THR	306	40.816	-5.616	84.428	1.00	43.35	A
ATOM	2153	O	THR	306	40.648	-4.883	85.405	1.00	44.14	A
ATOM	2154	N	PRO	307	41.944	-5.572	83.696	1.00	42.66	A
ATOM	2155	CD	PRO	307	42.230	-6.282	82.436	1.00	43.08	A
ATOM	2156	CA	PRO	307	43.039	-4.651	84.035	1.00	41.12	A
ATOM	2157	CB	PRO	307	44.109	-4.993	83.001	1.00	41.90	A
ATOM	2158	CG	PRO	307	43.302	-5.410	81.811	1.00	42.89	A
ATOM	2159	C	PRO	307	42.661	-3.165	84.023	1.00	39.78	A
ATOM	2160	O	PRO	307	43.151	-2.384	84.847	1.00	38.90	A
ATOM	2161	N	HIS	308	41.789	-2.773	83.099	1.00	36.76	A
ATOM	2162	CA	HIS	308	41.373	-1.381	83.018	1.00	34.24	A
ATOM	2163	CB	HIS	308	41.248	-0.946	81.558	1.00	35.68	A
ATOM	2164	CG	HIS	308	40.936	0.507	81.395	1.00	38.11	A
ATOM	2165	CD2	HIS	308	39.847	1.134	80.888	1.00	39.53	A
ATOM	2166	ND1	HIS	308	41.794	1.503	81.809	1.00	38.73	A
ATOM	2167	CE1	HIS	308	41.249	2.682	81.565	1.00	39.88	A
ATOM	2168	NE2	HIS	308	40.067	2.486	81.006	1.00	40.19	A
ATOM	2169	C	HIS	308	40.052	-1.120	83.737	1.00	31.65	A
ATOM	2170	O	HIS	308	39.009	-1.661	83.362	1.00	32.49	A
ATOM	2171	N	VAL	309	40.117	-0.282	84.769	1.00	26.89	A
ATOM	2172	CA	VAL	309	38.959	0.101	85.580	1.00	22.85	A
ATOM	2173	CB	VAL	309	39.298	-0.013	87.083	1.00	22.36	A
ATOM	2174	CG1	VAL	309	38.091	0.351	87.922	1.00	22.91	A
ATOM	2175	CG2	VAL	309	39.765	-1.427	87.403	1.00	22.12	A

ATOM	2176	C	VAL	309	38.629	1.558	85.231	1.00	20.44	A
ATOM	2177	O	VAL	309	39.450	2.446	85.433	1.00	19.97	A
ATOM	2178	N	PRO	310	37.421	1.822	84.704	1.00	17.91	A
ATOM	2179	CD	PRO	310	36.413	0.834	84.277	1.00	14.72	A
ATOM	2180	CA	PRO	310	37.019	3.186	84.322	1.00	17.34	A
ATOM	2181	CB	PRO	310	35.839	2.937	83.386	1.00	15.77	A
ATOM	2182	CG	PRO	310	35.214	1.699	83.978	1.00	15.26	A
ATOM	2183	C	PRO	310	36.689	4.227	85.404	1.00	16.65	A
ATOM	2184	O	PRO	310	35.673	4.908	85.317	1.00	15.99	A
ATOM	2185	N	TYR	311	37.557	4.368	86.402	1.00	18.31	A
ATOM	2186	CA	TYR	311	37.346	5.335	87.485	1.00	18.33	A
ATOM	2187	CB	TYR	311	38.549	5.374	88.430	1.00	18.13	A
ATOM	2188	CG	TYR	311	38.826	4.115	89.209	1.00	20.50	A
ATOM	2189	CD1	TYR	311	37.943	3.660	90.194	1.00	19.61	A
ATOM	2190	CE1	TYR	311	38.242	2.538	90.957	1.00	19.17	A
ATOM	2191	CD2	TYR	311	40.008	3.407	89.005	1.00	19.30	A
ATOM	2192	CE2	TYR	311	40.314	2.290	89.759	1.00	18.88	A
ATOM	2193	CZ	TYR	311	39.432	1.860	90.732	1.00	20.10	A
ATOM	2194	OH	TYR	311	39.754	0.749	91.480	1.00	23.13	A
ATOM	2195	C	TYR	311	37.150	6.753	86.969	1.00	19.65	A
ATOM	2196	O	TYR	311	36.288	7.485	87.449	1.00	20.71	A
ATOM	2197	N	ARG	312	37.967	7.140	85.995	1.00	19.46	A
ATOM	2198	CA	ARG	312	37.919	8.484	85.447	1.00	19.67	A
ATOM	2199	CB	ARG	312	39.223	8.775	84.699	1.00	24.48	A
ATOM	2200	CG	ARG	312	40.470	8.521	85.534	1.00	31.49	A
ATOM	2201	CD	ARG	312	41.737	8.793	84.742	1.00	38.21	A
ATOM	2202	NE	ARG	312	41.948	10.223	84.543	1.00	41.59	A
ATOM	2203	CZ	ARG	312	42.419	11.040	85.479	1.00	43.45	A
ATOM	2204	NH1	ARG	312	42.733	10.564	86.678	1.00	43.96	A
ATOM	2205	NH2	ARG	312	42.570	12.332	85.217	1.00	44.26	A
ATOM	2206	C	ARG	312	36.736	8.826	84.547	1.00	17.18	A
ATOM	2207	O	ARG	312	36.610	9.976	84.121	1.00	17.17	A
ATOM	2208	N	GLU	313	35.856	7.869	84.262	1.00	14.11	A
ATOM	2209	CA	GLU	313	34.729	8.178	83.378	1.00	11.27	A
ATOM	2210	CB	GLU	313	34.258	6.911	82.646	1.00	10.67	A
ATOM	2211	CG	GLU	313	35.399	6.213	81.891	1.00	15.89	A
ATOM	2212	CD	GLU	313	34.946	5.089	80.956	1.00	19.42	A
ATOM	2213	OE1	GLU	313	35.821	4.301	80.519	1.00	20.64	A
ATOM	2214	OE2	GLU	313	33.739	4.992	80.641	1.00	19.87	A
ATOM	2215	C	GLU	313	33.554	8.893	84.048	1.00	9.14	A
ATOM	2216	O	GLU	313	32.550	9.155	83.410	1.00	8.08	A
ATOM	2217	N	SER	314	33.692	9.226	85.327	1.00	9.25	A
ATOM	2218	CA	SER	314	32.647	9.951	86.051	1.00	11.62	A
ATOM	2219	CB	SER	314	31.508	9.011	86.467	1.00	14.09	A
ATOM	2220	OG	SER	314	31.812	8.354	87.688	1.00	14.04	A
ATOM	2221	C	SER	314	33.233	10.604	87.298	1.00	11.57	A
ATOM	2222	O	SER	314	34.283	10.186	87.791	1.00	12.89	A
ATOM	2223	N	LYS	315	32.541	11.615	87.812	1.00	12.14	A
ATOM	2224	CA	LYS	315	32.981	12.340	89.002	1.00	14.40	A
ATOM	2225	CB	LYS	315	32.082	13.556	89.246	1.00	17.33	A
ATOM	2226	CG	LYS	315	32.015	14.559	88.105	1.00	19.52	A
ATOM	2227	CD	LYS	315	33.175	15.536	88.143	1.00	22.04	A
ATOM	2228	CE	LYS	315	33.021	16.584	87.054	1.00	22.29	A
ATOM	2229	NZ	LYS	315	32.991	15.922	85.724	1.00	25.05	A
ATOM	2230	C	LYS	315	32.952	11.461	90.253	1.00	14.36	A
ATOM	2231	O	LYS	315	33.899	11.459	91.042	1.00	15.78	A
ATOM	2232	N	LEU	316	31.859	10.723	90.430	1.00	12.10	A
ATOM	2233	CA	LEU	316	31.693	9.864	91.591	1.00	12.11	A
ATOM	2234	CB	LEU	316	30.346	9.132	91.521	1.00	11.47	A
ATOM	2235	CG	LEU	316	30.052	8.165	92.673	1.00	11.12	A
ATOM	2236	CD1	LEU	316	29.755	8.941	93.947	1.00	10.52	A
ATOM	2237	CD2	LEU	316	28.867	7.294	92.313	1.00	9.92	A
ATOM	2238	C	LEU	316	32.816	8.846	91.790	1.00	12.47	A
ATOM	2239	O	LEU	316	33.346	8.720	92.892	1.00	13.63	A
ATOM	2240	N	THR	317	33.192	8.124	90.738	1.00	13.16	A
ATOM	2241	CA	THR	317	34.245	7.118	90.875	1.00	12.10	A
ATOM	2242	CB	THR	317	34.132	6.031	89.783	1.00	9.66	A
ATOM	2243	OG1	THR	317	34.077	6.642	88.496	1.00	9.89	A
ATOM	2244	CG2	THR	317	32.870	5.200	89.994	1.00	10.70	A
ATOM	2245	C	THR	317	35.674	7.681	90.923	1.00	12.84	A
ATOM	2246	O	THR	317	36.611	6.965	91.270	1.00	13.25	A
ATOM	2247	N	ARG	318	35.852	8.951	90.575	1.00	13.06	A
ATOM	2248	CA	ARG	318	37.180	9.544	90.682	1.00	14.05	A

ATOM	2249	CB	ARG	318	37.326	10.780	89.796	1.00	15.43	A
ATOM	2250	CG	ARG	318	37.417	10.473	88.319	1.00	20.15	A
ATOM	2251	CD	ARG	318	37.526	11.755	87.527	1.00	22.93	A
ATOM	2252	NE	ARG	318	38.747	12.468	87.865	1.00	27.97	A
ATOM	2253	CZ	ARG	318	39.015	13.710	87.482	1.00	32.10	A
ATOM	2254	NH1	ARG	318	38.138	14.383	86.747	1.00	32.47	A
ATOM	2255	NH2	ARG	318	40.162	14.276	87.833	1.00	33.23	A
ATOM	2256	C	ARG	318	37.281	9.948	92.138	1.00	13.35	A
ATOM	2257	O	ARG	318	38.276	9.679	92.801	1.00	15.31	A
ATOM	2258	N	ILE	319	36.222	10.575	92.640	1.00	12.79	A
ATOM	2259	CA	ILE	319	36.175	11.012	94.030	1.00	11.02	A
ATOM	2260	CB	ILE	319	34.837	11.727	94.322	1.00	9.24	A
ATOM	2261	CG2	ILE	319	34.660	11.958	95.819	1.00	4.84	A
ATOM	2262	CG1	ILE	319	34.786	13.047	93.561	1.00	9.26	A
ATOM	2263	CD1	ILE	319	33.431	13.786	93.692	1.00	9.14	A
ATOM	2264	C	ILE	319	36.344	9.833	95.002	1.00	12.21	A
ATOM	2265	O	ILE	319	37.127	9.913	95.950	1.00	12.33	A
ATOM	2266	N	LEU	320	35.627	8.739	94.752	1.00	10.74	A
ATOM	2267	CA	LEU	320	35.674	7.577	95.638	1.00	11.28	A
ATOM	2268	CB	LEU	320	34.240	7.142	95.965	1.00	8.50	A
ATOM	2269	CG	LEU	320	33.364	8.196	96.642	1.00	11.65	A
ATOM	2270	CD1	LEU	320	31.909	7.774	96.550	1.00	12.32	A
ATOM	2271	CD2	LEU	320	33.794	8.390	98.090	1.00	7.79	A
ATOM	2272	C	LEU	320	36.466	6.359	95.146	1.00	12.31	A
ATOM	2273	O	LEU	320	36.276	5.254	95.658	1.00	10.52	A
ATOM	2274	N	GLN	321	37.356	6.541	94.177	1.00	13.27	A
ATOM	2275	CA	GLN	321	38.110	5.401	93.668	1.00	16.08	A
ATOM	2276	CB	GLN	321	39.087	5.844	92.569	1.00	19.75	A
ATOM	2277	CG	GLN	321	40.196	6.756	93.006	1.00	21.68	A
ATOM	2278	CD	GLN	321	41.079	7.139	91.840	1.00	25.85	A
ATOM	2279	OE1	GLN	321	41.622	6.266	91.152	1.00	22.98	A
ATOM	2280	NE2	GLN	321	41.228	8.450	91.602	1.00	26.88	A
ATOM	2281	C	GLN	321	38.842	4.548	94.723	1.00	14.28	A
ATOM	2282	O	GLN	321	38.972	3.335	94.543	1.00	12.19	A
ATOM	2283	N	ASP	322	39.305	5.151	95.817	1.00	12.59	A
ATOM	2284	CA	ASP	322	39.978	4.351	96.835	1.00	14.78	A
ATOM	2285	CB	ASP	322	40.769	5.230	97.811	1.00	17.14	A
ATOM	2286	CG	ASP	322	41.787	4.426	98.620	1.00	18.36	A
ATOM	2287	OD1	ASP	322	42.588	3.692	98.003	1.00	19.34	A
ATOM	2288	OD2	ASP	322	41.791	4.521	99.865	1.00	19.68	A
ATOM	2289	C	ASP	322	38.988	3.473	97.609	1.00	15.66	A
ATOM	2290	O	ASP	322	39.384	2.598	98.384	1.00	17.16	A
ATOM	2291	N	SER	323	37.697	3.696	97.386	1.00	16.21	A
ATOM	2292	CA	SER	323	36.657	2.915	98.047	1.00	16.47	A
ATOM	2293	CB	SER	323	35.436	3.795	98.343	1.00	13.71	A
ATOM	2294	OG	SER	323	35.749	4.804	99.284	1.00	11.67	A
ATOM	2295	C	SER	323	36.247	1.735	97.166	1.00	18.02	A
ATOM	2296	O	SER	323	35.459	0.876	97.574	1.00	18.75	A
ATOM	2297	N	LEU	324	36.795	1.696	95.956	1.00	18.69	A
ATOM	2298	CA	LEU	324	36.495	0.635	95.009	1.00	19.76	A
ATOM	2299	CB	LEU	324	35.782	1.225	93.789	1.00	19.37	A
ATOM	2300	CG	LEU	324	34.461	1.920	94.127	1.00	19.69	A
ATOM	2301	CD1	LEU	324	34.028	2.781	92.973	1.00	22.50	A
ATOM	2302	CD2	LEU	324	33.394	0.887	94.449	1.00	20.33	A
ATOM	2303	C	LEU	324	37.789	-0.045	94.591	1.00	21.46	A
ATOM	2304	O	LEU	324	38.427	0.353	93.618	1.00	23.00	A
ATOM	2305	N	GLY	325	38.174	-1.074	95.341	1.00	22.77	A
ATOM	2306	CA	GLY	325	39.398	-1.794	95.047	1.00	21.76	A
ATOM	2307	C	GLY	325	40.620	-1.028	95.516	1.00	24.37	A
ATOM	2308	O	GLY	325	41.718	-1.239	95.005	1.00	24.93	A
ATOM	2309	N	GLY	326	40.428	-0.132	96.484	1.00	24.40	A
ATOM	2310	CA	GLY	326	41.526	0.663	97.002	1.00	24.15	A
ATOM	2311	C	GLY	326	41.897	0.284	98.424	1.00	26.42	A
ATOM	2312	O	GLY	326	41.656	-0.840	98.856	1.00	25.60	A
ATOM	2313	N	ARG	327	42.470	1.220	99.168	1.00	25.86	A
ATOM	2314	CA	ARG	327	42.875	0.919	100.528	1.00	28.96	A
ATOM	2315	CB	ARG	327	44.219	1.593	100.834	1.00	32.07	A
ATOM	2316	CG	ARG	327	45.329	1.220	99.853	1.00	37.14	A
ATOM	2317	CD	ARG	327	46.714	1.483	100.432	1.00	42.74	A
ATOM	2318	NE	ARG	327	47.800	1.031	99.556	1.00	47.24	A
ATOM	2319	CZ	ARG	327	48.286	1.730	98.530	1.00	49.78	A
ATOM	2320	NH1	ARG	327	47.787	2.926	98.237	1.00	50.77	A
ATOM	2321	NH2	ARG	327	49.286	1.245	97.805	1.00	49.64	A

ATOM	2322	C	ARG	327	41.831	1.320	101.569	1.00	28.96	A
ATOM	2323	O	ARG	327	42.157	1.543	102.731	1.00	28.88	A
ATOM	2324	N	THR	328	40.573	1.401	101.151	1.00	27.38	A
ATOM	2325	CA	THR	328	39.499	1.775	102.064	1.00	23.77	A
ATOM	2326	CB	THR	328	38.678	2.944	101.488	1.00	24.66	A
ATOM	2327	OG1	THR	328	39.529	4.088	101.344	1.00	25.37	A
ATOM	2328	CG2	THR	328	37.510	3.292	102.409	1.00	23.54	A
ATOM	2329	C	THR	328	38.556	0.611	102.353	1.00	20.49	A
ATOM	2330	O	THR	328	38.287	-0.213	101.480	1.00	19.13	A
ATOM	2331	N	ARG	329	38.072	0.532	103.588	1.00	17.06	A
ATOM	2332	CA	ARG	329	37.139	-0.522	103.954	1.00	15.33	A
ATOM	2333	CB	ARG	329	37.126	-0.768	105.465	1.00	14.79	A
ATOM	2334	CG	ARG	329	36.035	-1.748	105.878	1.00	15.14	A
ATOM	2335	CD	ARG	329	35.989	-2.023	107.370	1.00	17.09	A
ATOM	2336	NE	ARG	329	34.897	-2.947	107.655	1.00	21.72	A
ATOM	2337	CZ	ARG	329	34.688	-3.553	108.819	1.00	22.49	A
ATOM	2338	NH1	ARG	329	35.504	-3.343	109.841	1.00	20.08	A
ATOM	2339	NH2	ARG	329	33.646	-4.366	108.958	1.00	22.92	A
ATOM	2340	C	ARG	329	35.783	-0.001	103.539	1.00	14.65	A
ATOM	2341	O	ARG	329	35.352	1.046	104.030	1.00	15.12	A
ATOM	2342	N	THR	330	35.107	-0.704	102.640	1.00	12.06	A
ATOM	2343	CA	THR	330	33.809	-0.226	102.224	1.00	14.04	A
ATOM	2344	CB	THR	330	33.837	0.332	100.782	1.00	15.17	A
ATOM	2345	OG1	THR	330	33.694	-0.735	99.847	1.00	18.22	A
ATOM	2346	CG2	THR	330	35.147	1.052	100.513	1.00	14.36	A
ATOM	2347	C	THR	330	32.707	-1.265	102.323	1.00	13.65	A
ATOM	2348	O	THR	330	32.936	-2.459	102.140	1.00	13.67	A
ATOM	2349	N	SER	331	31.509	-0.786	102.637	1.00	12.70	A
ATOM	2350	CA	SER	331	30.340	-1.627	102.740	1.00	10.49	A
ATOM	2351	CB	SER	331	29.830	-1.648	104.177	1.00	12.02	A
ATOM	2352	OG	SER	331	30.860	-2.026	105.072	1.00	18.36	A
ATOM	2353	C	SER	331	29.259	-1.044	101.830	1.00	10.83	A
ATOM	2354	O	SER	331	29.235	0.160	101.555	1.00	8.62	A
ATOM	2355	N	ILE	332	28.376	-1.906	101.349	1.00	9.52	A
ATOM	2356	CA	ILE	332	27.288	-1.457	100.511	1.00	9.50	A
ATOM	2357	CB	ILE	332	27.374	-2.038	99.089	1.00	10.70	A
ATOM	2358	CG2	ILE	332	26.143	-1.622	98.287	1.00	8.05	A
ATOM	2359	CG1	ILE	332	28.650	-1.560	98.394	1.00	9.17	A
ATOM	2360	CD1	ILE	332	28.773	-2.094	96.975	1.00	5.23	A
ATOM	2361	C	ILE	332	25.993	-1.939	101.138	1.00	9.51	A
ATOM	2362	O	ILE	332	25.843	-3.127	101.413	1.00	9.19	A
ATOM	2363	N	ILE	333	25.074	-1.015	101.391	1.00	9.81	A
ATOM	2364	CA	ILE	333	23.773	-1.376	101.942	1.00	8.92	A
ATOM	2365	CB	ILE	333	23.335	-0.444	103.103	1.00	8.82	A
ATOM	2366	CG2	ILE	333	21.967	-0.863	103.614	1.00	7.93	A
ATOM	2367	CG1	ILE	333	24.316	-0.548	104.272	1.00	6.76	A
ATOM	2368	CD1	ILE	333	24.028	0.448	105.387	1.00	2.97	A
ATOM	2369	C	ILE	333	22.777	-1.240	100.797	1.00	9.34	A
ATOM	2370	O	ILE	333	22.483	-0.132	100.347	1.00	6.58	A
ATOM	2371	N	ALA	334	22.294	-2.376	100.303	1.00	9.13	A
ATOM	2372	CA	ALA	334	21.325	-2.370	99.215	1.00	8.43	A
ATOM	2373	CB	ALA	334	21.543	-3.582	98.318	1.00	6.36	A
ATOM	2374	C	ALA	334	19.903	-2.381	99.807	1.00	8.65	A
ATOM	2375	O	ALA	334	19.555	-3.232	100.634	1.00	6.98	A
ATOM	2376	N	THR	335	19.089	-1.419	99.398	1.00	8.61	A
ATOM	2377	CA	THR	335	17.727	-1.334	99.899	1.00	8.77	A
ATOM	2378	CB	THR	335	17.375	0.092	100.290	1.00	7.57	A
ATOM	2379	OG1	THR	335	17.538	0.949	99.157	1.00	8.21	A
ATOM	2380	CG2	THR	335	18.276	0.552	101.398	1.00	7.82	A
ATOM	2381	C	THR	335	16.729	-1.820	98.863	1.00	8.70	A
ATOM	2382	O	THR	335	16.855	-1.530	97.671	1.00	8.21	A
ATOM	2383	N	ILE	336	15.735	-2.560	99.338	1.00	8.74	A
ATOM	2384	CA	ILE	336	14.717	-3.124	98.469	1.00	10.87	A
ATOM	2385	CB	ILE	336	14.998	-4.613	98.216	1.00	10.46	A
ATOM	2386	CG2	ILE	336	16.353	-4.769	97.532	1.00	8.62	A
ATOM	2387	CG1	ILE	336	14.943	-5.379	99.543	1.00	10.60	A
ATOM	2388	CD1	ILE	336	14.993	-6.921	99.386	1.00	10.91	A
ATOM	2389	C	ILE	336	13.291	-2.995	99.004	1.00	12.03	A
ATOM	2390	O	ILE	336	13.069	-2.844	100.204	1.00	12.49	A
ATOM	2391	N	SER	337	12.331	-3.056	98.089	1.00	13.93	A
ATOM	2392	CA	SER	337	10.918	-2.969	98.426	1.00	13.83	A
ATOM	2393	CB	SER	337	10.180	-2.154	97.359	1.00	14.05	A
ATOM	2394	OG	SER	337	8.790	-2.436	97.350	1.00	13.32	A

ATOM	2395	C	SER	337	10.371	-4.386	98.464	1.00	14.60	A
ATOM	2396	O	SER	337	10.829	-5.250	97.717	1.00	14.95	A
ATOM	2397	N	PRO	338	9.398	-4.652	99.350	1.00	15.93	A
ATOM	2398	CD	PRO	338	8.967	-3.811	100.483	1.00	16.39	A
ATOM	2399	CA	PRO	338	8.809	-5.990	99.451	1.00	15.42	A
ATOM	2400	CB	PRO	338	8.461	-6.088	100.921	1.00	15.52	A
ATOM	2401	CG	PRO	338	7.930	-4.705	101.176	1.00	17.59	A
ATOM	2402	C	PRO	338	7.564	-6.138	98.576	1.00	15.52	A
ATOM	2403	O	PRO	338	6.929	-7.185	98.571	1.00	17.10	A
ATOM	2404	N	ALA	339	7.212	-5.091	97.841	1.00	15.73	A
ATOM	2405	CA	ALA	339	6.023	-5.122	96.989	1.00	17.08	A
ATOM	2406	CB	ALA	339	5.494	-3.699	96.765	1.00	13.90	A
ATOM	2407	C	ALA	339	6.255	-5.793	95.647	1.00	17.79	A
ATOM	2408	O	ALA	339	7.290	-5.586	95.010	1.00	18.27	A
ATOM	2409	N	SER	340	5.270	-6.575	95.210	1.00	19.26	A
ATOM	2410	CA	SER	340	5.339	-7.280	93.933	1.00	20.19	A
ATOM	2411	CB	SER	340	4.088	-8.151	93.741	1.00	21.56	A
ATOM	2412	OG	SER	340	2.909	-7.370	93.812	1.00	24.50	A
ATOM	2413	C	SER	340	5.495	-6.340	92.736	1.00	18.83	A
ATOM	2414	O	SER	340	5.977	-6.755	91.687	1.00	17.98	A
ATOM	2415	N	LEU	341	5.083	-5.084	92.883	1.00	19.49	A
ATOM	2416	CA	LEU	341	5.212	-4.114	91.793	1.00	21.42	A
ATOM	2417	CB	LEU	341	4.539	-2.787	92.159	1.00	24.24	A
ATOM	2418	CG	LEU	341	3.056	-2.763	92.528	1.00	30.57	A
ATOM	2419	CD1	LEU	341	2.838	-3.310	93.952	1.00	30.86	A
ATOM	2420	CD2	LEU	341	2.563	-1.325	92.435	1.00	32.23	A
ATOM	2421	C	LEU	341	6.678	-3.821	91.452	1.00	20.58	A
ATOM	2422	O	LEU	341	7.017	-3.528	90.308	1.00	20.62	A
ATOM	2423	N	ASN	342	7.544	-3.905	92.455	1.00	19.46	A
ATOM	2424	CA	ASN	342	8.958	-3.620	92.267	1.00	18.47	A
ATOM	2425	CB	ASN	342	9.471	-2.863	93.485	1.00	17.34	A
ATOM	2426	CG	ASN	342	8.662	-1.618	93.763	1.00	16.86	A
ATOM	2427	OD1	ASN	342	8.564	-0.730	92.916	1.00	18.67	A
ATOM	2428	ND2	ASN	342	8.070	-1.546	94.944	1.00	15.28	A
ATOM	2429	C	ASN	342	9.795	-4.871	92.041	1.00	18.85	A
ATOM	2430	O	ASN	342	10.988	-4.893	92.351	1.00	17.91	A
ATOM	2431	N	LEU	343	9.170	-5.908	91.493	1.00	17.20	A
ATOM	2432	CA	LEU	343	9.863	-7.163	91.252	1.00	17.19	A
ATOM	2433	CB	LEU	343	8.917	-8.179	90.596	1.00	13.78	A
ATOM	2434	CG	LEU	343	9.593	-9.472	90.107	1.00	14.61	A
ATOM	2435	CD1	LEU	343	10.343	-10.143	91.269	1.00	10.55	A
ATOM	2436	CD2	LEU	343	8.554	-10.415	89.499	1.00	13.10	A
ATOM	2437	C	LEU	343	11.115	-7.020	90.399	1.00	17.48	A
ATOM	2438	O	LEU	343	12.211	-7.377	90.829	1.00	17.34	A
ATOM	2439	N	GLU	344	10.946	-6.514	89.184	1.00	19.72	A
ATOM	2440	CA	GLU	344	12.063	-6.358	88.263	1.00	20.96	A
ATOM	2441	CB	GLU	344	11.598	-5.684	86.969	1.00	24.20	A
ATOM	2442	CG	GLU	344	12.675	-5.635	85.887	1.00	32.62	A
ATOM	2443	CD	GLU	344	12.213	-4.959	84.599	1.00	38.13	A
ATOM	2444	OE1	GLU	344	12.908	-5.115	83.566	1.00	40.01	A
ATOM	2445	OE2	GLU	344	11.165	-4.270	84.617	1.00	41.47	A
ATOM	2446	C	GLU	344	13.208	-5.561	88.883	1.00	20.19	A
ATOM	2447	O	GLU	344	14.371	-5.957	88.791	1.00	20.32	A
ATOM	2448	N	GLU	345	12.883	-4.441	89.518	1.00	17.74	A
ATOM	2449	CA	GLU	345	13.909	-3.615	90.130	1.00	18.84	A
ATOM	2450	CB	GLU	345	13.335	-2.240	90.496	1.00	21.25	A
ATOM	2451	CG	GLU	345	13.076	-1.356	89.281	1.00	24.52	A
ATOM	2452	CD	GLU	345	14.348	-1.036	88.492	1.00	27.03	A
ATOM	2453	OE1	GLU	345	14.232	-0.592	87.325	1.00	29.83	A
ATOM	2454	OE2	GLU	345	15.462	-1.216	89.036	1.00	27.61	A
ATOM	2455	C	GLU	345	14.555	-4.270	91.346	1.00	16.79	A
ATOM	2456	O	GLU	345	15.762	-4.143	91.554	1.00	17.33	A
ATOM	2457	N	THR	346	13.760	-4.978	92.140	1.00	14.42	A
ATOM	2458	CA	THR	346	14.286	-5.649	93.316	1.00	14.40	A
ATOM	2459	CB	THR	346	13.160	-6.304	94.138	1.00	15.55	A
ATOM	2460	OG1	THR	346	12.399	-5.285	94.801	1.00	13.04	A
ATOM	2461	CG2	THR	346	13.735	-7.255	95.171	1.00	15.14	A
ATOM	2462	C	THR	346	15.302	-6.705	92.896	1.00	14.50	A
ATOM	2463	O	THR	346	16.294	-6.922	93.590	1.00	13.63	A
ATOM	2464	N	LEU	347	15.061	-7.362	91.763	1.00	14.51	A
ATOM	2465	CA	LEU	347	16.005	-8.357	91.269	1.00	15.49	A
ATOM	2466	CB	LEU	347	15.369	-9.222	90.167	1.00	15.24	A
ATOM	2467	CG	LEU	347	14.220	-10.158	90.571	1.00	15.51	A

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ATOM   2468  CD1 LEU   347      13.712 -10.902  89.351  1.00 11.90      A
ATOM   2469  CD2 LEU   347      14.687 -11.142  91.627  1.00 13.17      A
ATOM   2470  C   LEU   347      17.267  -7.666  90.734  1.00 16.52      A
ATOM   2471  O   LEU   347      18.376  -8.175  90.908  1.00 18.79      A
ATOM   2472  N   SER   348      17.111  -6.513  90.088  1.00 15.74      A
ATOM   2473  CA  SER   348      18.274  -5.795  89.567  1.00 16.97      A
ATOM   2474  CB  SER   348      17.857  -4.502  88.872  1.00 17.03      A
ATOM   2475  OG  SER   348      17.008  -4.785  87.780  1.00 23.78      A
ATOM   2476  C   SER   348      19.199  -5.438  90.712  1.00 16.29      A
ATOM   2477  O   SER   348      20.415  -5.668  90.655  1.00 17.03      A
ATOM   2478  N   THR   349      18.603  -4.864  91.751  1.00 13.43      A
ATOM   2479  CA  THR   349      19.341  -4.452  92.925  1.00 12.53      A
ATOM   2480  CB  THR   349      18.400  -3.808  93.953  1.00 11.53      A
ATOM   2481  OG1 THR   349      17.883  -2.583  93.416  1.00 12.14      A
ATOM   2482  CG2 THR   349      19.143  -3.512  95.243  1.00  8.21      A
ATOM   2483  C   THR   349      20.074  -5.624  93.563  1.00 12.73      A
ATOM   2484  O   THR   349      21.292  -5.590  93.732  1.00 10.74      A
ATOM   2485  N   LEU   350      19.325  -6.660  93.916  1.00 14.33      A
ATOM   2486  CA  LEU   350      19.923  -7.830  94.532  1.00 16.65      A
ATOM   2487  CB  LEU   350      18.855  -8.892  94.803  1.00 14.51      A
ATOM   2488  CG  LEU   350      17.916  -8.537  95.960  1.00 13.75      A
ATOM   2489  CD1 LEU   350      16.780  -9.516  96.035  1.00 10.80      A
ATOM   2490  CD2 LEU   350      18.703  -8.526  97.258  1.00 15.25      A
ATOM   2491  C   LEU   350      21.033  -8.400  93.660  1.00 17.62      A
ATOM   2492  O   LEU   350      22.116  -8.695  94.148  1.00 19.69      A
ATOM   2493  N   GLU   351      20.774  -8.540  92.368  1.00 18.77      A
ATOM   2494  CA  GLU   351      21.783  -9.078  91.466  1.00 20.26      A
ATOM   2495  CB  GLU   351      21.203  -9.215  90.061  1.00 23.16      A
ATOM   2496  CG  GLU   351      21.961 -10.194  89.186  1.00 31.07      A
ATOM   2497  CD  GLU   351      21.645 -11.652  89.508  1.00 35.15      A
ATOM   2498  OE1 GLU   351      22.421 -12.531  89.070  1.00 37.94      A
ATOM   2499  OE2 GLU   351      20.621 -11.921  90.180  1.00 35.11      A
ATOM   2500  C   GLU   351      23.030  -8.181  91.440  1.00 18.73      A
ATOM   2501  O   GLU   351      24.163  -8.662  91.407  1.00 18.86      A
ATOM   2502  N   TYR   352      22.810  -6.873  91.463  1.00 18.82      A
ATOM   2503  CA  TYR   352      23.893  -5.898  91.443  1.00 16.90      A
ATOM   2504  CB  TYR   352      23.304  -4.500  91.261  1.00 17.28      A
ATOM   2505  CG  TYR   352      24.306  -3.374  91.118  1.00 15.30      A
ATOM   2506  CD1 TYR   352      24.940  -2.833  92.227  1.00 12.89      A
ATOM   2507  CE1 TYR   352      25.779  -1.740  92.100  1.00 15.82      A
ATOM   2508  CD2 TYR   352      24.550  -2.798  89.869  1.00 15.34      A
ATOM   2509  CE2 TYR   352      25.382  -1.712  89.731  1.00 14.65      A
ATOM   2510  CZ  TYR   352      25.989  -1.180  90.848  1.00 15.26      A
ATOM   2511  OH  TYR   352      26.767  -0.050  90.715  1.00 17.76      A
ATOM   2512  C   TYR   352      24.688  -5.973  92.733  1.00 16.43      A
ATOM   2513  O   TYR   352      25.917  -5.964  92.715  1.00 17.51      A
ATOM   2514  N   ALA   353      23.989  -6.065  93.855  1.00 15.81      A
ATOM   2515  CA  ALA   353      24.658  -6.137  95.145  1.00 16.65      A
ATOM   2516  CB  ALA   353      23.646  -5.931  96.269  1.00 15.23      A
ATOM   2517  C   ALA   353      25.405  -7.458  95.350  1.00 17.40      A
ATOM   2518  O   ALA   353      26.412  -7.497  96.050  1.00 18.96      A
ATOM   2519  N   HIS   354      24.916  -8.535  94.744  1.00 18.26      A
ATOM   2520  CA  HIS   354      25.555  -9.838  94.883  1.00 19.76      A
ATOM   2521  CB  HIS   354      24.676 -10.932  94.266  1.00 19.50      A
ATOM   2522  CG  HIS   354      25.143 -12.324  94.566  1.00 21.21      A
ATOM   2523  CD2 HIS   354      25.758 -13.246  93.786  1.00 20.11      A
ATOM   2524  ND1 HIS   354      25.032 -12.894  95.817  1.00 20.61      A
ATOM   2525  CE1 HIS   354      25.561 -14.105  95.796  1.00 20.62      A
ATOM   2526  NE2 HIS   354      26.009 -14.342  94.576  1.00 20.83      A
ATOM   2527  C   HIS   354      26.936  -9.842  94.224  1.00 21.08      A
ATOM   2528  O   HIS   354      27.903 -10.313  94.816  1.00 22.05      A
ATOM   2529  N   ARG   355      27.027  -9.314  93.004  1.00 22.49      A
ATOM   2530  CA  ARG   355      28.308  -9.256  92.292  1.00 24.62      A
ATOM   2531  CB  ARG   355      28.153  -8.619  90.905  1.00 25.83      A
ATOM   2532  CG  ARG   355      27.358  -9.413  89.894  1.00 29.38      A
ATOM   2533  CD  ARG   355      27.482  -8.762  88.535  1.00 32.38      A
ATOM   2534  NE  ARG   355      27.233  -7.326  88.622  1.00 37.22      A
ATOM   2535  CZ  ARG   355      27.902  -6.412  87.924  1.00 40.93      A
ATOM   2536  NH1 ARG   355      28.860  -6.797  87.087  1.00 41.58      A
ATOM   2537  NH2 ARG   355      27.624  -5.117  88.066  1.00 39.72      A
ATOM   2538  C   ARG   355      29.352  -8.447  93.054  1.00 24.34      A
ATOM   2539  O   ARG   355      30.523  -8.821  93.098  1.00 25.69      A
ATOM   2540  N   ALA   356      28.923  -7.332  93.640  1.00 23.36      A
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ATOM	2541	CA	ALA	356	29.814	-6.447	94.387	1.00	22.82	A
ATOM	2542	CB	ALA	356	29.016	-5.295	94.985	1.00	20.20	A
ATOM	2543	C	ALA	356	30.603	-7.161	95.484	1.00	23.12	A
ATOM	2544	O	ALA	356	31.708	-6.751	95.820	1.00	20.69	A
ATOM	2545	N	LYS	357	30.030	-8.222	96.047	1.00	24.95	A
ATOM	2546	CA	LYS	357	30.695	-8.981	97.111	1.00	26.72	A
ATOM	2547	CB	LYS	357	29.849	-10.195	97.497	1.00	25.95	A
ATOM	2548	CG	LYS	357	28.570	-9.854	98.232	1.00	27.20	A
ATOM	2549	CD	LYS	357	27.647	-11.052	98.293	1.00	28.41	A
ATOM	2550	CE	LYS	357	28.288	-12.220	99.024	1.00	29.67	A
ATOM	2551	NZ	LYS	357	27.537	-13.483	98.790	1.00	30.65	A
ATOM	2552	C	LYS	357	32.099	-9.453	96.733	1.00	27.68	A
ATOM	2553	O	LYS	357	32.968	-9.595	97.601	1.00	26.10	A
ATOM	2554	N	ASN	358	32.312	-9.691	95.438	1.00	28.56	A
ATOM	2555	CA	ASN	358	33.591	-10.177	94.925	1.00	28.98	A
ATOM	2556	CB	ASN	358	33.363	-10.897	93.597	1.00	31.13	A
ATOM	2557	CG	ASN	358	32.415	-12.071	93.735	1.00	34.60	A
ATOM	2558	OD1	ASN	358	32.743	-13.071	94.375	1.00	37.20	A
ATOM	2559	ND2	ASN	358	31.226	-11.952	93.145	1.00	33.97	A
ATOM	2560	C	ASN	358	34.676	-9.118	94.751	1.00	27.98	A
ATOM	2561	O	ASN	358	35.784	-9.426	94.316	1.00	28.50	A
ATOM	2562	N	ILE	359	34.364	-7.871	95.079	1.00	25.92	A
ATOM	2563	CA	ILE	359	35.350	-6.811	94.957	1.00	24.09	A
ATOM	2564	CB	ILE	359	34.673	-5.429	94.910	1.00	21.25	A
ATOM	2565	CG2	ILE	359	35.727	-4.329	94.867	1.00	19.17	A
ATOM	2566	CG1	ILE	359	33.748	-5.367	93.689	1.00	19.08	A
ATOM	2567	CD1	ILE	359	32.909	-4.109	93.597	1.00	18.25	A
ATOM	2568	C	ILE	359	36.290	-6.906	96.155	1.00	25.26	A
ATOM	2569	O	ILE	359	35.847	-7.076	97.290	1.00	23.96	A
ATOM	2570	N	LEU	360	37.588	-6.817	95.897	1.00	27.58	A
ATOM	2571	CA	LEU	360	38.578	-6.917	96.963	1.00	32.07	A
ATOM	2572	CB	LEU	360	39.478	-8.137	96.722	1.00	34.40	A
ATOM	2573	CG	LEU	360	40.711	-8.333	97.613	1.00	36.57	A
ATOM	2574	CD1	LEU	360	40.309	-8.930	98.961	1.00	37.87	A
ATOM	2575	CD2	LEU	360	41.687	-9.265	96.913	1.00	38.48	A
ATOM	2576	C	LEU	360	39.438	-5.665	97.033	1.00	33.54	A
ATOM	2577	O	LEU	360	39.905	-5.174	96.008	1.00	32.97	A
ATOM	2578	N	ASN	361	39.635	-5.132	98.234	1.00	35.62	A
ATOM	2579	CA	ASN	361	40.485	-3.962	98.372	1.00	39.86	A
ATOM	2580	CB	ASN	361	39.649	-2.672	98.395	1.00	41.32	A
ATOM	2581	CG	ASN	361	38.490	-2.732	99.345	1.00	42.28	A
ATOM	2582	OD1	ASN	361	37.523	-1.985	99.203	1.00	42.60	A
ATOM	2583	ND2	ASN	361	38.578	-3.609	100.330	1.00	45.41	A
ATOM	2584	C	ASN	361	41.439	-4.056	99.565	1.00	41.68	A
ATOM	2585	O	ASN	361	41.180	-4.768	100.532	1.00	41.90	A
ATOM	2586	N	LYS	362	42.560	-3.348	99.446	1.00	44.89	A
ATOM	2587	CA	LYS	362	43.643	-3.321	100.432	1.00	46.74	A
ATOM	2588	CB	LYS	362	43.106	-3.372	101.870	1.00	45.91	A
ATOM	2589	CG	LYS	362	42.518	-2.057	102.353	1.00	44.95	A
ATOM	2590	CD	LYS	362	42.184	-2.089	103.841	1.00	44.77	A
ATOM	2591	CE	LYS	362	43.444	-2.056	104.701	1.00	44.68	A
ATOM	2592	NZ	LYS	362	44.224	-0.795	104.523	1.00	44.09	A
ATOM	2593	C	LYS	362	44.576	-4.504	100.173	1.00	48.88	A
ATOM	2594	O	LYS	362	44.928	-5.219	101.141	1.00	50.91	A
ATOM	2595	OXT	LYS	362	44.955	-4.700	98.992	1.00	49.21	A
ATOM	2596	MG	MG	603	16.038	9.381	98.154	1.00	22.45	
ATOM	2597	PB	ADP	601	14.871	6.512	98.896	1.00	9.83	ADP
ATOM	2598	O1B	ADP	601	14.389	7.073	97.604	1.00	11.43	ADP
ATOM	2599	O2B	ADP	601	15.417	5.029	98.682	1.00	12.43	ADP
ATOM	2600	O3B	ADP	601	15.921	7.374	99.491	1.00	9.54	ADP
ATOM	2601	PA	ADP	601	13.343	7.143	101.254	1.00	13.34	ADP
ATOM	2602	O1A	ADP	601	14.336	6.832	102.280	1.00	14.02	ADP
ATOM	2603	O2A	ADP	601	13.336	8.581	101.013	1.00	12.22	ADP
ATOM	2604	O3A	ADP	601	13.676	6.373	99.912	1.00	11.56	ADP
ATOM	2605	O5*	ADP	601	11.879	6.778	101.742	1.00	16.31	ADP
ATOM	2606	C5*	ADP	601	10.894	5.934	101.155	1.00	16.15	ADP
ATOM	2607	C4*	ADP	601	9.662	5.974	102.132	1.00	18.96	ADP
ATOM	2608	O4*	ADP	601	9.712	4.734	102.849	1.00	19.62	ADP
ATOM	2609	C3*	ADP	601	9.700	7.065	103.229	1.00	18.60	ADP
ATOM	2610	O3*	ADP	601	8.406	7.650	103.431	1.00	22.72	ADP
ATOM	2611	C2*	ADP	601	10.188	6.391	104.496	1.00	19.66	ADP
ATOM	2612	O2*	ADP	601	9.655	6.994	105.672	1.00	21.78	ADP
ATOM	2613	C1*	ADP	601	9.788	4.947	104.281	1.00	19.08	ADP

ATOM	2614	N9	ADP	601	10.778	3.943	104.795	1.00	19.36	ADP	
ATOM	2615	C8	ADP	601	11.895	3.536	104.137	1.00	19.33	ADP	
ATOM	2616	N7	ADP	601	12.535	2.641	104.859	1.00	19.29	ADP	
ATOM	2617	C5	ADP	601	11.874	2.450	105.961	1.00	20.60	ADP	
ATOM	2618	C6	ADP	601	12.043	1.649	107.091	1.00	20.38	ADP	
ATOM	2619	N6	ADP	601	13.085	0.825	107.178	1.00	20.28	ADP	
ATOM	2620	N1	ADP	601	11.118	1.701	108.120	1.00	22.79	ADP	
ATOM	2621	C2	ADP	601	10.028	2.524	108.081	1.00	22.78	ADP	
ATOM	2622	N3	ADP	601	9.854	3.302	106.988	1.00	20.98	ADP	
ATOM	2623	C4	ADP	601	10.736	3.301	105.936	1.00	20.39	ADP	
ATOM	2859	C1	5-2b	2	19.000	14.175	112.199	1.00	28.18	5-2b	
ATOM	2860	C2	5-2b	2	18.061	13.539	111.340	1.00	32.48	5-2b	
ATOM	2861	C3	5-2b	2	17.078	12.651	111.895	1.00	28.56	5-2b	
ATOM	2862	C4	5-2b	2	17.088	12.427	113.305	1.00	27.05	5-2b	
ATOM	2863	C5	5-2b	2	18.039	13.044	114.157	1.00	26.16	5-2b	
ATOM	2864	C6	5-2b	2	19.015	13.950	113.622	1.00	28.62	5-2b	
ATOM	2865	C7	5-2b	2	18.128	13.723	109.878	1.00	39.58	5-2b	
ATOM	2866	N8	5-2b	2	19.295	13.211	109.173	1.00	34.03	5-2b	
ATOM	2867	C9	5-2b	2	20.221	14.007	108.603	1.00	31.92	5-2b	
ATOM	2868	N10	5-2b	2	19.947	15.297	108.469	1.00	36.78	5-2b	
ATOM	2869	C11	5-2b	2	18.661	15.862	108.801	1.00	44.76	5-2b	
ATOM	2870	C12	5-2b	2	17.708	15.078	109.368	1.00	52.53	5-2b	
ATOM	2871	O13	5-2b	2	16.238	11.708	113.800	1.00	23.44	5-2b	
ATOM	2872	C14	5-2b	2	16.264	15.498	109.536	1.00	70.42	5-2b	
ATOM	2873	O15	5-2b	2	15.927	16.837	109.475	1.00	104.53	5-2b	
ATOM	2874	C16	5-2b	2	14.579	17.475	109.627	1.00	95.04	5-2b	
ATOM	2875	C17	5-2b	2	14.646	19.021	109.575	1.00	97.91	5-2b	
ATOM	2876	C18	5-2b	2	18.590	17.336	108.468	1.00	43.13	5-2b	
ATOM	2877	O19	5-2b	2	15.462	14.612	109.721	1.00	72.50	5-2b	
ATOM	2878	S20	5-2b	2	21.688	13.451	108.038	1.00	18.17	5-2b	
ATOM	2624	O	HOH	1	20.805	10.444	96.618	1.00	3.59	S	
ATOM	2625	O	HOH	6	18.478	8.895	97.954	1.00	22.75	S	
ATOM	2626	O	HOH	7	8.678	16.203	114.749	1.00	5.86	S	
ATOM	2627	O	HOH	8	15.946	-1.691	94.899	1.00	5.80	S	
ATOM	2628	O	HOH	11	21.220	17.072	106.339	1.00	1.72	S	
ATOM	2629	O	HOH	13	14.805	10.449	99.917	1.00	8.07	S	
ATOM	2630	O	HOH	16	13.355	-2.493	95.064	1.00	7.03	S	
ATOM	2631	O	HOH	19	21.262	3.695	111.999	1.00	8.18	S	
ATOM	2632	O	HOH	20	10.684	13.846	117.065	1.00	18.83	S	
ATOM	2633	O	HOH	25	21.216	2.976	93.758	1.00	14.00	S	
ATOM	2634	O	HOH	27	24.932	11.371	102.192	1.00	7.13	S	
ATOM	2635	O	HOH	34	15.711	22.783	114.948	1.00	8.16	S	
ATOM	2636	O	HOH	35	31.658	6.477	79.773	1.00	16.68	S	
ATOM	2637	O	HOH	36	16.262	7.930	95.115	1.00	13.14	S	
ATOM	2638	O	HOH	38	15.341	-0.450	103.081	1.00	3.96	S	
ATOM	2639	O	HOH	40	20.527	12.061	101.135	1.00	13.66	S	
ATOM	2640	O	HOH	42	31.548	4.510	82.184	1.00	13.63	S	
ATOM	2641	O	HOH	44	20.139	3.415	109.317	1.00	9.63	S	
ATOM	2642	O	HOH	46	38.748	2.216	117.615	1.00	16.12	S	
ATOM	2643	O	HOH	48	37.332	6.832	98.871	1.00	20.54	S	
ATOM	2644	O	HOH	50	15.243	1.107	105.237	1.00	7.71	S	
ATOM	2645	O	HOH	52	23.362	13.594	103.308	1.00	16.03	S	
ATOM	2646	O	HOH	54	24.373	1.678	79.508	1.00	21.19	S	
ATOM	2647	O	HOH	55	38.272	4.890	80.366	1.00	15.34	S	
ATOM	2648	O	HOH	60	28.231	24.639	95.411	1.00	10.59	S	
ATOM	2649	O	HOH	61	39.120	8.121	96.836	1.00	17.30	S	
ATOM	2650	O	HOH	63	18.805	15.804	105.109	1.00	24.81	S	
ATOM	2651	O	HOH	64	40.943	11.048	89.550	1.00	24.53	S	
ATOM	2652	O	HOH	68	31.035	20.952	88.723	1.00	17.53	S	
ATOM	2653	O	HOH	69	19.610	-3.671	118.241	1.00	28.77	S	
ATOM	2654	O	HOH	70	23.256	19.519	117.749	1.00	12.03	S	
ATOM	2655	O	HOH	71	21.279	14.920	97.265	1.00	17.07	S	
ATOM	2656	O	HOH	72	11.571	8.465	98.099	1.00	17.54	S	
ATOM	2657	O	HOH	73	0.219	-7.157	96.638	1.00	36.34	S	
ATOM	2658	O	HOH	74	14.061	-2.365	107.352	1.00	17.49	S	
ATOM	2659	O	HOH	75	38.428	6.714	101.400	1.00	20.61	S	
ATOM	2660	O	HOH	76	28.147	6.297	79.763	1.00	6.93	S	
ATOM	2661	O	HOH	78	16.520	-15.702	110.664	1.00	42.69	S	
ATOM	2662	O	HOH	79	40.740	11.793	96.499	1.00	19.31	S	
ATOM	2663	O	HOH	82	38.334	-6.005	104.252	1.00	25.92	S	
ATOM	2664	O	HOH	83	28.296	4.768	77.136	1.00	31.56	S	
ATOM	2665	O	HOH	84	14.008	16.450	94.704	1.00	5.75	S	
ATOM	2666	O	HOH	87	45.629	7.251	110.783	1.00	17.29	S	

ATOM	2667	O	HOH	90	13.592	18.093	92.309	1.00	13.66	S
ATOM	2668	O	HOH	91	9.122	2.181	96.091	1.00	36.98	S
ATOM	2669	O	HOH	92	16.369	12.885	106.048	1.00	20.85	S
ATOM	2670	O	HOH	93	13.386	21.050	89.915	1.00	17.97	S
ATOM	2671	O	HOH	94	11.913	22.331	96.952	1.00	21.35	S
ATOM	2672	O	HOH	95	20.093	-2.163	89.951	1.00	16.99	S
ATOM	2673	O	HOH	96	17.551	-0.999	87.296	1.00	26.38	S
ATOM	2674	O	HOH	97	20.767	15.478	84.877	1.00	51.52	S
ATOM	2675	O	HOH	99	35.477	1.749	79.785	1.00	19.87	S
ATOM	2676	O	HOH	101	21.955	8.778	118.594	1.00	28.07	S
ATOM	2677	O	HOH	102	40.041	5.064	84.678	1.00	16.03	S
ATOM	2678	O	HOH	104	36.377	-3.662	102.275	1.00	18.75	S
ATOM	2679	O	HOH	106	3.852	11.665	120.058	1.00	30.71	S
ATOM	2680	O	HOH	108	39.673	-0.150	74.200	1.00	46.52	S
ATOM	2681	O	HOH	110	6.144	-12.000	92.235	1.00	50.82	S
ATOM	2682	O	HOH	111	30.628	20.566	102.526	1.00	21.67	S
ATOM	2683	O	HOH	112	30.065	26.389	96.506	1.00	17.19	S
ATOM	2684	O	HOH	113	14.004	8.985	104.371	1.00	25.20	S
ATOM	2685	O	HOH	114	33.791	0.715	74.652	1.00	19.53	S
ATOM	2686	O	HOH	117	22.111	19.027	120.746	1.00	38.73	S
ATOM	2687	O	HOH	118	26.607	0.227	84.656	1.00	17.38	S
ATOM	2688	O	HOH	121	21.035	-9.445	110.275	1.00	13.05	S
ATOM	2689	O	HOH	122	32.184	14.826	101.349	1.00	11.39	S
ATOM	2690	O	HOH	123	17.599	-1.616	90.813	1.00	13.59	S
ATOM	2691	O	HOH	124	34.130	25.646	110.137	1.00	23.55	S
ATOM	2692	O	HOH	126	9.990	-6.133	95.389	1.00	15.79	S
ATOM	2693	O	HOH	129	3.202	-12.862	94.601	1.00	59.83	S
ATOM	2694	O	HOH	130	13.955	10.696	95.694	1.00	19.43	S
ATOM	2695	O	HOH	131	31.703	25.858	98.664	1.00	24.88	S
ATOM	2696	O	HOH	132	35.057	22.912	85.606	1.00	40.74	S
ATOM	2697	O	HOH	134	15.475	-7.722	86.631	1.00	12.20	S
ATOM	2698	O	HOH	135	17.594	16.623	102.663	1.00	23.55	S
ATOM	2699	O	HOH	136	7.395	-14.251	99.064	1.00	49.69	S
ATOM	2700	O	HOH	137	16.245	22.597	107.873	1.00	19.89	S
ATOM	2701	O	HOH	139	9.431	-0.664	90.038	1.00	31.01	S
ATOM	2702	O	HOH	145	19.183	30.020	93.555	1.00	40.54	S
ATOM	2703	O	HOH	146	27.383	12.738	122.250	1.00	22.34	S
ATOM	2704	O	HOH	148	39.078	-6.174	93.184	1.00	34.51	S
ATOM	2705	O	HOH	149	49.726	3.941	96.574	1.00	41.42	S
ATOM	2706	O	HOH	151	13.531	20.213	113.505	1.00	35.47	S
ATOM	2707	O	HOH	152	49.848	18.275	102.636	1.00	39.85	S
ATOM	2708	O	HOH	153	27.728	-14.666	103.176	1.00	32.11	S
ATOM	2709	O	HOH	154	17.610	7.968	89.633	1.00	32.29	S
ATOM	2710	O	HOH	155	16.723	19.937	85.776	1.00	24.59	S
ATOM	2711	O	HOH	158	31.015	-3.720	75.821	1.00	31.57	S
ATOM	2712	O	HOH	159	39.461	15.014	103.524	1.00	34.83	S
ATOM	2713	O	HOH	164	45.236	2.614	116.065	1.00	33.66	S
ATOM	2714	O	HOH	166	28.893	5.418	123.561	1.00	30.64	S
ATOM	2715	O	HOH	167	35.887	12.107	99.622	1.00	11.12	S
ATOM	2716	O	HOH	168	29.323	-10.874	107.683	1.00	39.92	S
ATOM	2717	O	HOH	170	33.078	22.456	122.206	1.00	27.20	S
ATOM	2718	O	HOH	171	6.377	-23.385	91.461	1.00	39.35	S
ATOM	2719	O	HOH	175	38.059	24.742	100.957	1.00	44.52	S
ATOM	2720	O	HOH	179	12.119	-0.723	109.488	1.00	28.60	S
ATOM	2721	O	HOH	184	35.206	-9.022	104.290	1.00	21.93	S
ATOM	2722	O	HOH	186	5.690	-6.930	88.872	1.00	26.18	S
ATOM	2723	O	HOH	187	3.662	-13.329	100.868	1.00	25.44	S
ATOM	2724	O	HOH	188	8.547	-5.057	88.499	1.00	31.53	S
ATOM	2725	O	HOH	189	13.396	13.012	123.817	1.00	23.03	S
ATOM	2726	O	HOH	190	37.857	10.497	99.808	1.00	16.10	S
ATOM	2727	O	HOH	191	15.390	0.870	75.556	1.00	32.35	S
ATOM	2728	O	HOH	192	24.877	12.484	84.150	1.00	33.77	S
ATOM	2729	O	HOH	195	7.560	1.921	103.939	1.00	24.38	S
ATOM	2730	O	HOH	197	38.275	6.762	75.942	1.00	34.75	S
ATOM	2731	O	HOH	198	11.981	14.135	109.242	1.00	26.93	S
ATOM	2732	O	HOH	199	29.034	-13.318	94.699	1.00	32.78	S
ATOM	2733	O	HOH	201	33.413	-10.638	103.290	1.00	31.96	S
ATOM	2734	O	HOH	203	25.859	12.342	87.393	1.00	39.56	S
ATOM	2735	O	HOH	205	21.304	4.617	78.647	1.00	17.67	S
ATOM	2736	O	HOH	207	23.255	12.937	88.372	1.00	28.66	S
ATOM	2737	O	HOH	208	7.965	2.363	93.256	1.00	39.90	S
ATOM	2738	O	HOH	210	7.291	-19.119	97.337	1.00	39.55	S
ATOM	2739	O	HOH	211	23.200	15.157	105.669	1.00	3.65	S

ATOM	2740	O	HOH	212	16.820	11.748	98.364	1.00	4.40	S
ATOM	2741	O	HOH	215	37.029	15.874	102.172	1.00	9.34	S
ATOM	2742	O	HOH	217	45.218	10.237	90.158	1.00	50.32	S
ATOM	2743	O	HOH	220	46.617	4.288	108.402	1.00	29.26	S
ATOM	2744	O	HOH	221	18.955	8.984	95.378	1.00	23.41	S
ATOM	2745	O	HOH	223	22.905	6.137	118.403	1.00	15.81	S
ATOM	2746	O	HOH	225	2.959	-6.265	97.196	1.00	46.93	S
ATOM	2747	O	HOH	226	11.436	16.916	109.490	1.00	15.86	S
ATOM	2748	O	HOH	228	16.698	14.117	102.916	1.00	25.42	S
ATOM	2749	O	HOH	229	14.674	21.461	106.079	1.00	26.44	S
ATOM	2750	O	HOH	232	21.595	-5.809	87.827	1.00	14.15	S
ATOM	2751	O	HOH	233	11.151	17.123	115.185	1.00	32.57	S
ATOM	2752	O	HOH	238	29.371	-3.075	77.740	1.00	19.94	S
ATOM	2753	O	HOH	241	13.508	12.891	99.625	1.00	20.34	S
ATOM	2754	O	HOH	243	17.423	4.974	118.567	1.00	24.32	S
ATOM	2755	O	HOH	244	21.246	6.736	82.924	1.00	39.07	S
ATOM	2756	O	HOH	245	11.590	19.689	98.284	1.00	19.24	S
ATOM	2757	O	HOH	247	51.802	9.068	117.095	1.00	55.38	S
ATOM	2758	O	HOH	251	8.180	5.024	99.128	1.00	31.61	S
ATOM	2759	O	HOH	252	21.300	12.368	98.575	1.00	31.29	S
ATOM	2760	O	HOH	253	41.894	8.695	97.607	1.00	30.47	S
ATOM	2761	O	HOH	254	23.625	0.733	121.375	1.00	27.92	S
ATOM	2762	O	HOH	255	29.438	14.355	123.667	1.00	26.17	S
ATOM	2763	O	HOH	256	20.446	10.316	116.657	1.00	34.15	S
ATOM	2764	O	HOH	257	11.975	9.878	91.516	1.00	18.84	S
ATOM	2765	O	HOH	260	13.789	3.056	113.975	1.00	23.75	S
ATOM	2766	O	HOH	262	7.623	13.572	124.008	1.00	30.74	S
ATOM	2767	O	HOH	263	20.395	4.227	81.694	1.00	33.87	S
ATOM	2768	O	HOH	266	34.255	-0.467	81.343	1.00	30.08	S
ATOM	2769	O	HOH	268	45.417	1.198	105.917	1.00	33.79	S
ATOM	2770	O	HOH	271	15.540	-18.971	104.185	1.00	36.81	S
ATOM	2771	O	HOH	272	31.560	28.306	95.365	1.00	25.41	S
ATOM	2772	O	HOH	273	10.820	11.774	124.773	1.00	27.96	S
ATOM	2773	O	HOH	275	16.259	16.032	106.228	1.00	15.83	S
ATOM	2774	O	HOH	279	14.255	23.209	104.198	1.00	21.24	S
ATOM	2775	O	HOH	280	14.152	22.369	109.944	1.00	30.26	S
ATOM	2776	O	HOH	281	28.645	-13.914	110.927	1.00	35.08	S
ATOM	2777	O	HOH	283	15.855	18.951	102.400	1.00	31.06	S
ATOM	2778	O	HOH	288	15.557	2.812	116.261	1.00	19.13	S
ATOM	2779	O	HOH	290	52.550	19.096	99.218	1.00	47.57	S
ATOM	2780	O	HOH	291	26.202	14.680	81.794	1.00	53.97	S
ATOM	2781	O	HOH	294	20.086	20.598	120.312	1.00	37.20	S
ATOM	2782	O	HOH	295	6.012	19.892	120.875	1.00	18.20	S
ATOM	2783	O	HOH	296	30.916	30.335	103.939	1.00	37.71	S
ATOM	2784	O	HOH	297	46.048	18.195	120.452	1.00	43.25	S
ATOM	2785	O	HOH	299	31.569	-9.610	101.042	1.00	32.15	S
ATOM	2786	O	HOH	300	21.162	-3.401	87.125	1.00	32.61	S
ATOM	2787	O	HOH	303	9.761	2.577	112.502	1.00	27.58	S
ATOM	2788	O	HOH	305	32.066	25.918	112.422	1.00	32.24	S
ATOM	2789	O	HOH	307	33.480	-2.576	83.015	1.00	27.49	S
ATOM	2790	O	HOH	308	2.984	13.923	120.708	1.00	31.57	S
ATOM	2791	O	HOH	309	34.596	-15.790	94.772	1.00	43.06	S
ATOM	2792	O	HOH	310	34.476	-4.326	104.147	1.00	46.76	S
ATOM	2793	O	HOH	313	18.109	-9.045	87.036	1.00	25.07	S
ATOM	2794	O	HOH	314	2.837	9.810	121.659	1.00	42.28	S
ATOM	2795	O	HOH	315	13.698	1.784	111.141	1.00	35.74	S
ATOM	2796	O	HOH	317	34.111	18.005	122.006	1.00	28.52	S
ATOM	2797	O	HOH	318	29.111	-3.283	83.701	1.00	38.21	S
ATOM	2798	O	HOH	319	32.667	0.553	105.431	1.00	27.32	S
ATOM	2799	O	HOH	323	4.556	-19.468	88.447	1.00	56.20	S
ATOM	2800	O	HOH	324	-2.283	-4.890	97.004	1.00	48.36	S
ATOM	2801	O	HOH	327	28.636	-3.285	118.234	1.00	30.32	S
ATOM	2802	O	HOH	328	29.441	25.536	120.010	1.00	30.29	S
ATOM	2803	O	HOH	331	25.024	1.315	88.662	1.00	35.16	S
ATOM	2804	O	HOH	332	25.076	33.728	92.315	1.00	37.36	S
ATOM	2805	O	HOH	334	17.967	17.125	84.628	1.00	44.99	S
ATOM	2806	O	HOH	336	35.277	-4.775	82.255	1.00	22.90	S
ATOM	2807	O	HOH	338	5.655	-0.231	95.494	1.00	39.33	S
ATOM	2808	O	HOH	340	46.414	-2.129	108.144	1.00	58.72	S
ATOM	2809	O	HOH	342	10.262	-2.840	88.835	1.00	36.82	S
ATOM	2810	O	HOH	344	48.378	-0.812	102.187	1.00	39.43	S
ATOM	2811	O	HOH	345	7.840	6.837	118.967	1.00	54.06	S
ATOM	2812	O	HOH	347	42.036	-0.811	90.785	1.00	34.08	S

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ATOM   2813  O   HOH   351      51.775   6.542 133.541  1.00 37.45      S
ATOM   2814  O   HOH   354      31.545  13.101  83.668  1.00 37.78      S
ATOM   2815  O   HOH   355      35.526  14.686 100.364  1.00  8.84      S
ATOM   2816  O   HOH   361      12.290  20.796 107.012  1.00 17.59      S
ATOM   2817  O   HOH   363      40.627   4.272 127.391  1.00 41.84      S
ATOM   2818  O   HOH   365      30.371  -1.879  79.833  1.00 13.67      S
ATOM   2819  O   HOH   367      11.687  18.291 107.264  1.00 22.06      S
ATOM   2820  O   HOH   370      18.511   7.004 119.773  1.00 38.47      S
ATOM   2821  O   HOH   371      17.908  13.463 100.054  1.00 12.12      S
ATOM   2822  O   HOH   372      27.131  -3.005  76.310  1.00 16.74      S
ATOM   2823  O   HOH   375       8.972   7.528  97.923  1.00 26.11      S
ATOM   2824  O   HOH   377      18.727  10.788  84.519  1.00 41.33      S
ATOM   2825  O   HOH   379      14.127  15.750  98.863  1.00 25.29      S
ATOM   2826  O   HOH   383      41.700   9.858  81.807  1.00 33.52      S
ATOM   2827  O   HOH   385      35.261  15.280 106.016  1.00 28.87      S
ATOM   2828  O   HOH   386      12.726  21.661 115.689  1.00 46.81      S
ATOM   2829  O   HOH   393      43.648   7.839 106.741  1.00 16.47      S
ATOM   2830  O   HOH   394      37.259  24.740 104.054  1.00 14.17      S
ATOM   2831  O   HOH   396      24.282  -6.502  87.829  1.00 42.62      S
ATOM   2832  O   HOH   400      43.027  -3.036  92.095  1.00 34.87      S
ATOM   2833  O   HOH   406      31.066  -3.244  81.803  1.00 24.95      S
ATOM   2834  O   HOH   409      36.251   3.079 119.019  1.00 19.28      S
ATOM   2835  O   HOH   415      10.534  10.025 100.073  1.00 39.35      S
ATOM   2836  O   HOH   418       8.054   4.181 110.289  1.00 45.64      S
ATOM   2837  O   HOH   422      39.306  16.744 111.576  1.00 34.28      S
ATOM   2838  O   HOH   425       6.396   5.427 103.157  1.00 32.56      S
ATOM   2839  O   HOH   426      39.952  24.546  98.144  1.00 27.08      S
ATOM   2840  O   HOH   429      39.863   6.685  82.133  1.00 40.09      S
ATOM   2841  O   HOH   430      21.921  12.487  85.799  1.00 40.68      S
ATOM   2842  O   HOH   433      11.505  19.654 100.809  1.00 30.56      S
ATOM   2843  O   HOH   435      10.302  11.568 104.901  1.00 29.96      S
ATOM   2844  O   HOH   438      23.476  -0.876  78.128  1.00 28.68      S
ATOM   2845  O   HOH   442      40.869  23.992 100.914  1.00 39.98      S
ATOM   2846  O   HOH   444      36.147  28.207  94.921  1.00 46.43      S
ATOM   2847  O   HOH   445      23.713   3.771 119.077  1.00 42.21      S
ATOM   2848  O   HOH   447      27.306  -4.631  90.698  1.00 43.77      S
ATOM   2849  O   HOH   448      45.805   6.819 107.875  1.00 28.04      S
ATOM   2850  O   HOH   449      11.162   9.197 125.577  1.00 42.08      S
ATOM   2851  O   HOH   450      51.897   9.884 132.993  1.00 37.33      S
ATOM   2852  O   HOH   452      28.491   3.721 119.002  1.00 32.94      S
ATOM   2853  O   HOH   454       8.173  10.098 105.141  1.00 50.50      S
ATOM   2854  O   HOH   459      42.750   5.736  87.519  1.00 36.93      S
ATOM   2855  O   HOH   460      30.376  34.460  94.131  1.00 31.43      S
ATOM   2856  O   HOH   466      25.986   1.393 120.060  1.00 52.81      S
ATOM   2857  O   HOH   467      22.489 -10.959 108.669  1.00 29.27      S
ATOM   2858  O   HOH   468      23.362  -2.077  86.180  1.00 37.76      S
END
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TABLE 2

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REMARK   1 Compound 1-7_3dpb.pdb molecule B
!CRYST   69.250   79.750  159.580  90.00  90.00  90.00 P212121
ATOM     20  CB  LYS    17      24.352 -12.458  60.280  1.00 51.00      B
ATOM     21  CG  LYS    17      22.874 -12.492  59.882  1.00 53.34      B
ATOM     22  CD  LYS    17      22.663 -12.316  58.375  1.00 53.77      B
ATOM     23  CE  LYS    17      23.197 -13.512  57.582  1.00 54.85      B
ATOM     24  NZ  LYS    17      24.682 -13.693  57.700  1.00 53.86      B
ATOM     25  C   LYS    17      24.606 -10.105  59.443  1.00 47.83      B
ATOM     26  O   LYS    17      25.275 -10.140  58.419  1.00 48.69      B
ATOM     27  N   LYS    17      24.345 -10.549  61.888  1.00 49.93      B
ATOM     28  CA  LYS    17      24.911 -11.048  60.601  1.00 49.15      B
ATOM     29  N   ASN    18      23.597  -9.260  59.599  1.00 45.98      B
ATOM     30  CA  ASN    18      23.245  -8.340  58.535  1.00 43.66      B
ATOM     31  CB  ASN    18      21.960  -7.627  58.880  1.00 45.49      B
ATOM     32  CG  ASN    18      20.740  -8.481  58.599  1.00 49.80      B
ATOM     33  OD1 ASN    18      20.453  -8.811  57.442  1.00 50.22      B
ATOM     34  ND2 ASN    18      20.019  -8.856  59.653  1.00 49.94      B
ATOM     35  C   ASN    18      24.338  -7.336  58.180  1.00 41.30      B
ATOM     36  O   ASN    18      24.671  -7.173  57.006  1.00 41.62      B
ATOM     37  N   ILE    19      24.906  -6.669  59.179  1.00 37.77      B
ATOM     38  CA  ILE    19      25.949  -5.679  58.928  1.00 34.25      B
ATOM     39  CB  ILE    19      26.325  -4.966  60.253  1.00 35.25      B
ATOM     40  CG2 ILE    19      26.548  -5.988  61.346  1.00 38.29      B
ATOM     41  CG1 ILE    19      27.581  -4.139  60.078  1.00 35.22      B
ATOM     42  CD1 ILE    19      28.042  -3.487  61.347  1.00 36.16      B
ATOM     43  C   ILE    19      27.213  -6.272  58.266  1.00 31.28      B
ATOM     44  O   ILE    19      27.730  -7.287  58.722  1.00 31.52      B
ATOM     45  N   GLN    20      27.699  -5.639  57.194  1.00 27.50      B
ATOM     46  CA  GLN    20      28.903  -6.091  56.483  1.00 26.14      B
ATOM     47  CB  GLN    20      28.889  -5.603  54.996  1.00 25.10      B
ATOM     48  CG  GLN    20      30.276  -5.495  54.347  1.00 27.01      B
ATOM     49  CD  GLN    20      30.232  -5.169  52.843  1.00 29.81      B
ATOM     50  OE1 GLN    20      29.920  -6.026  52.016  1.00 30.67      B
ATOM     51  NE2 GLN    20      30.546  -3.924  52.493  1.00 30.62      B
ATOM     52  C   GLN    20      30.162  -5.567  57.176  1.00 25.43      B
ATOM     53  O   GLN    20      30.211  -4.398  57.561  1.00 27.09      B
ATOM     54  N   VAL    21      31.176  -6.426  57.327  1.00 22.08      B
ATOM     55  CA  VAL    21      32.427  -6.048  57.989  1.00 18.37      B
ATOM     56  CB  VAL    21      32.472  -6.584  59.471  1.00 19.87      B
ATOM     57  CG1 VAL    21      33.802  -6.230  60.125  1.00 16.85      B
ATOM     58  CG2 VAL    21      31.300  -6.004  60.291  1.00 14.97      B
ATOM     59  C   VAL    21      33.648  -6.567  57.221  1.00 18.19      B
ATOM     60  O   VAL    21      33.848  -7.771  57.081  1.00 16.60      B
ATOM     61  N   VAL    22      34.457  -5.637  56.722  1.00 17.58      B
ATOM     62  CA  VAL    22      35.651  -5.965  55.967  1.00 15.68      B
ATOM     63  CB  VAL    22      35.568  -5.385  54.532  1.00 17.56      B
ATOM     64  CG1 VAL    22      34.305  -5.889  53.846  1.00 17.79      B
ATOM     65  CG2 VAL    22      35.553  -3.863  54.575  1.00 17.41      B
ATOM     66  C   VAL    22      36.869  -5.396  56.693  1.00 16.43      B
ATOM     67  O   VAL    22      36.746  -4.502  57.549  1.00 14.89      B
ATOM     68  N   VAL    23      38.038  -5.936  56.358  1.00 14.83      B
ATOM     69  CA  VAL    23      39.304  -5.534  56.972  1.00 13.82      B
ATOM     70  CB  VAL    23      39.935  -6.745  57.768  1.00 13.54      B
ATOM     71  CG1 VAL    23      41.330  -6.405  58.282  1.00  6.83      B
ATOM     72  CG2 VAL    23      39.034  -7.112  58.944  1.00 13.12      B
ATOM     73  C   VAL    23      40.304  -5.023  55.928  1.00 13.37      B
ATOM     74  O   VAL    23      40.414  -5.576  54.835  1.00 10.49      B
ATOM     75  N   ARG    24      41.008  -3.944  56.256  1.00 14.76      B
ATOM     76  CA  ARG    24      42.019  -3.407  55.346  1.00 17.25      B
ATOM     77  CB  ARG    24      41.577  -2.087  54.700  1.00 14.29      B
ATOM     78  CG  ARG    24      42.528  -1.660  53.590  1.00 12.98      B
ATOM     79  CD  ARG    24      42.331  -0.225  53.130  1.00  9.77      B
ATOM     80  NE  ARG    24      42.978  -0.006  51.838  1.00  9.97      B
ATOM     81  CZ  ARG    24      42.881   1.111  51.112  1.00  9.72      B
ATOM     82  NH1 ARG    24      42.165   2.143  51.544  1.00  3.96      B
ATOM     83  NH2 ARG    24      43.477   1.177  49.923  1.00  8.75      B
ATOM     84  C   ARG    24      43.328  -3.180  56.098  1.00 18.12      B
ATOM     85  O   ARG    24      43.384  -2.408  57.055  1.00 16.79      B
ATOM     86  N   CYS    25      44.372  -3.874  55.657  1.00 21.17      B
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ATOM     87  CA  CYS    25      45.688  -3.764  56.268  1.00 23.23      B
ATOM     88  CB  CYS    25      46.415  -5.140  56.254  1.00 23.67      B
ATOM     89  SG  CYS    25      48.096  -5.149  56.970  1.00 28.58      B
ATOM     90  C   CYS    25      46.464  -2.764  55.443  1.00 24.61      B
ATOM     91  O   CYS    25      46.457  -2.836  54.211  1.00 24.46      B
ATOM     92  N   ARG    26      47.116  -1.818  56.109  1.00 25.36      B
ATOM     93  CA  ARG    26      47.897  -0.829  55.380  1.00 27.69      B
ATOM     94  CB  ARG    26      48.087   0.458  56.219  1.00 26.88      B
ATOM     95  CG  ARG    26      49.165   0.361  57.300  1.00 25.37      B
ATOM     96  CD  ARG    26      49.817   1.722  57.544  1.00 26.81      B
ATOM     97  NE  ARG    26      51.181   1.599  58.060  1.00 30.34      B
ATOM     98  CZ  ARG    26      51.504   1.598  59.349  1.00 31.91      B
ATOM     99  NH1 ARG    26      50.566   1.721  60.277  1.00 32.84      B
ATOM    100  NH2 ARG    26      52.767   1.459  59.714  1.00 33.10      B
ATOM    101  C   ARG    26      49.268  -1.423  55.072  1.00 29.73      B
ATOM    102  O   ARG    26      49.673  -2.417  55.676  1.00 28.95      B
ATOM    103  N   PRO    27      49.991  -0.832  54.108  1.00 31.27      B
ATOM    104  CD  PRO    27      49.498   0.108  53.083  1.00 32.66      B
ATOM    105  CA  PRO    27      51.327  -1.324  53.757  1.00 32.62      B
ATOM    106  CB  PRO    27      51.452  -0.937  52.287  1.00 31.65      B
ATOM    107  CG  PRO    27      50.745   0.369  52.235  1.00 31.82      B
ATOM    108  C   PRO    27      52.372  -0.626  54.642  1.00 33.24      B
ATOM    109  O   PRO    27      52.065   0.364  55.311  1.00 33.16      B
ATOM    110  N   PHE    28      53.599  -1.141  54.652  1.00 34.79      B
ATOM    111  CA  PHE    28      54.670  -0.545  55.451  1.00 34.86      B
ATOM    112  CB  PHE    28      55.890  -1.393  55.401  1.00 33.35      B
ATOM    113  CG  PHE    28      55.756  -2.691  56.124  1.00 33.06      B
ATOM    114  CD1 PHE    28      55.856  -3.893  55.440  1.00 31.63      B
ATOM    115  CD2 PHE    28      55.590  -2.715  57.507  1.00 31.31      B
ATOM    116  CE1 PHE    28      55.801  -5.102  56.128  1.00 31.40      B
ATOM    117  CE2 PHE    28      55.536  -3.918  58.193  1.00 30.69      B
ATOM    118  CZ  PHE    28      55.644  -5.112  57.500  1.00 29.86      B
ATOM    119  C   PHE    28      55.043   0.842  54.956  1.00 36.62      B
ATOM    120  O   PHE    28      55.102   1.080  53.752  1.00 36.72      B
ATOM    121  N   ASN    29      55.297   1.755  55.885  1.00 39.15      B
ATOM    122  CA  ASN    29      55.687   3.109  55.517  1.00 43.00      B
ATOM    123  CB  ASN    29      55.449   4.078  56.693  1.00 41.82      B
ATOM    124  CG  ASN    29      55.787   3.460  58.044  1.00 41.11      B
ATOM    125  OD1 ASN    29      56.953   3.237  58.367  1.00 38.49      B
ATOM    126  ND2 ASN    29      54.758   3.178  58.838  1.00 40.06      B
ATOM    127  C   ASN    29      57.160   3.083  55.130  1.00 46.95      B
ATOM    128  O   ASN    29      57.913   2.236  55.621  1.00 48.65      B
ATOM    129  N   LEU    30      57.554   3.998  54.243  1.00 49.22      B
ATOM    130  CA  LEU    30      58.930   4.106  53.751  1.00 49.70      B
ATOM    131  CB  LEU    30      59.142   5.490  53.121  1.00 49.24      B
ATOM    132  CG  LEU    30      60.429   5.757  52.341  1.00 49.29      B
ATOM    133  CD1 LEU    30      60.294   7.104  51.640  1.00 49.07      B
ATOM    134  CD2 LEU    30      61.643   5.740  53.264  1.00 49.24      B
ATOM    135  C   LEU    30      59.989   3.866  54.823  1.00 51.07      B
ATOM    136  O   LEU    30      60.877   3.032  54.649  1.00 50.68      B
ATOM    137  N   ALA    31      59.889   4.605  55.925  1.00 52.87      B
ATOM    138  CA  ALA    31      60.831   4.497  57.035  1.00 54.80      B
ATOM    139  CB  ALA    31      60.399   5.420  58.157  1.00 53.50      B
ATOM    140  C   ALA    31      61.011   3.077  57.576  1.00 56.55      B
ATOM    141  O   ALA    31      62.140   2.649  57.837  1.00 56.62      B
ATOM    142  N   GLU    32      59.906   2.354  57.751  1.00 59.00      B
ATOM    143  CA  GLU    32      59.958   0.989  58.272  1.00 61.92      B
ATOM    144  CB  GLU    32      58.625   0.631  58.999  1.00 61.49      B
ATOM    145  CG  GLU    32      57.413   0.441  58.094  1.00 60.80      B
ATOM    146  CD  GLU    32      56.101   0.376  58.872  1.00 59.87      B
ATOM    147  OE1 GLU    32      55.038   0.196  58.242  1.00 58.45      B
ATOM    148  OE2 GLU    32      56.129   0.514  60.115  1.00 60.23      B
ATOM    149  C   GLU    32      60.270  -0.057  57.198  1.00 64.49      B
ATOM    150  O   GLU    32      60.610  -1.199  57.522  1.00 64.33      B
ATOM    151  N   ARG    33      60.148   0.330  55.927  1.00 67.16      B
ATOM    152  CA  ARG    33      60.447  -0.573  54.813  1.00 69.70      B
ATOM    153  CB  ARG    33      59.996   0.033  53.435  1.00 71.95      B
ATOM    154  CG  ARG    33      58.567   0.570  53.353  1.00 75.31      B
ATOM    155  CD  ARG    33      58.383   1.377  52.056  1.00 78.38      B
ATOM    156  NE  ARG    33      57.203   2.248  52.066  1.00 80.30      B
ATOM    157  CZ  ARG    33      56.937   3.167  51.136  1.00 80.67      B
ATOM    158  NH1 ARG    33      57.766   3.345  50.114  1.00 79.70      B
ATOM    159  NH2 ARG    33      55.841   3.913  51.226  1.00 80.30      B
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ATOM	160	C	ARG	33	61.965	-0.720	54.794	1.00	70.18	B
ATOM	161	O	ARG	33	62.502	-1.813	54.599	1.00	70.13	B
ATOM	162	N	LYS	34	62.638	0.411	54.997	1.00	70.20	B
ATOM	163	CA	LYS	34	64.094	0.483	55.012	1.00	70.34	B
ATOM	164	CB	LYS	34	64.552	1.980	55.063	1.00	71.26	B
ATOM	165	CG	LYS	34	66.041	2.209	54.795	1.00	71.67	B
ATOM	166	CD	LYS	34	66.407	3.688	54.868	1.00	71.50	B
ATOM	167	CE	LYS	34	66.116	4.260	56.251	1.00	72.55	B
ATOM	168	NZ	LYS	34	66.513	5.694	56.388	1.00	72.95	B
ATOM	169	C	LYS	34	64.644	-0.288	56.211	1.00	70.18	B
ATOM	170	O	LYS	34	65.707	-0.915	56.123	1.00	70.68	B
ATOM	171	N	ALA	35	63.921	-0.236	57.330	1.00	68.80	B
ATOM	172	CA	ALA	35	64.324	-0.952	58.540	1.00	67.64	B
ATOM	173	CB	ALA	35	63.605	-0.381	59.760	1.00	67.24	B
ATOM	174	C	ALA	35	63.958	-2.424	58.356	1.00	66.54	B
ATOM	175	O	ALA	35	64.075	-3.232	59.286	1.00	65.43	B
ATOM	176	N	SER	36	63.520	-2.750	57.138	1.00	64.95	B
ATOM	177	CA	SER	36	63.113	-4.099	56.770	1.00	63.77	B
ATOM	178	CB	SER	36	64.347	-4.974	56.532	1.00	63.33	B
ATOM	179	OG	SER	36	65.136	-4.438	55.481	1.00	61.84	B
ATOM	180	C	SER	36	62.240	-4.670	57.879	1.00	63.32	B
ATOM	181	O	SER	36	62.731	-5.313	58.810	1.00	63.79	B
ATOM	182	N	ALA	37	60.939	-4.417	57.772	1.00	61.85	B
ATOM	183	CA	ALA	37	59.989	-4.873	58.773	1.00	59.96	B
ATOM	184	CB	ALA	37	58.921	-3.806	58.987	1.00	59.90	B
ATOM	185	C	ALA	37	59.344	-6.219	58.442	1.00	58.87	B
ATOM	186	O	ALA	37	58.975	-6.499	57.301	1.00	58.65	B
ATOM	187	N	HIS	38	59.215	-7.038	59.479	1.00	57.20	B
ATOM	188	CA	HIS	38	58.638	-8.378	59.411	1.00	54.48	B
ATOM	189	CB	HIS	38	59.315	-9.263	60.513	1.00	56.18	B
ATOM	190	CG	HIS	38	59.436	-8.582	61.851	1.00	56.74	B
ATOM	191	CD2	HIS	38	59.058	-8.977	63.092	1.00	57.32	B
ATOM	192	ND1	HIS	38	60.024	-7.344	62.011	1.00	55.67	B
ATOM	193	CE1	HIS	38	60.005	-7.006	63.288	1.00	56.12	B
ATOM	194	NE2	HIS	38	59.424	-7.980	63.967	1.00	57.53	B
ATOM	195	C	HIS	38	57.118	-8.352	59.615	1.00	51.90	B
ATOM	196	O	HIS	38	56.642	-8.343	60.754	1.00	52.05	B
ATOM	197	N	SER	39	56.356	-8.350	58.523	1.00	47.82	B
ATOM	198	CA	SER	39	54.893	-8.320	58.619	1.00	44.47	B
ATOM	199	CB	SER	39	54.255	-8.336	57.219	1.00	43.58	B
ATOM	200	OG	SER	39	52.837	-8.377	57.305	1.00	37.62	B
ATOM	201	C	SER	39	54.303	-9.468	59.435	1.00	43.06	B
ATOM	202	O	SER	39	54.681	-10.624	59.246	1.00	42.78	B
ATOM	203	N	ILE	40	53.373	-9.144	60.334	1.00	41.07	B
ATOM	204	CA	ILE	40	52.727	-10.162	61.157	1.00	39.33	B
ATOM	205	CB	ILE	40	52.660	-9.761	62.665	1.00	39.17	B
ATOM	206	CG2	ILE	40	54.063	-9.542	63.215	1.00	38.53	B
ATOM	207	CG1	ILE	40	51.824	-8.511	62.858	1.00	39.67	B
ATOM	208	CD1	ILE	40	51.496	-8.238	64.319	1.00	38.82	B
ATOM	209	C	ILE	40	51.314	-10.456	60.663	1.00	38.28	B
ATOM	210	O	ILE	40	50.591	-11.249	61.265	1.00	37.83	B
ATOM	211	N	VAL	41	50.932	-9.837	59.550	1.00	38.34	B
ATOM	212	CA	VAL	41	49.597	-10.047	59.000	1.00	38.90	B
ATOM	213	CB	VAL	41	48.792	-8.724	58.956	1.00	39.34	B
ATOM	214	CG1	VAL	41	47.421	-8.971	58.345	1.00	38.41	B
ATOM	215	CG2	VAL	41	48.648	-8.154	60.360	1.00	38.28	B
ATOM	216	C	VAL	41	49.535	-10.683	57.612	1.00	38.55	B
ATOM	217	O	VAL	41	50.184	-10.243	56.661	1.00	36.24	B
ATOM	218	N	GLU	42	48.728	-11.729	57.513	1.00	40.08	B
ATOM	219	CA	GLU	42	48.528	-12.433	56.255	1.00	42.70	B
ATOM	220	CB	GLU	42	48.931	-13.916	56.393	1.00	45.52	B
ATOM	221	CG	GLU	42	50.403	-14.215	56.163	1.00	47.68	B
ATOM	222	CD	GLU	42	50.783	-15.636	56.578	1.00	50.75	B
ATOM	223	OE1	GLU	42	49.991	-16.576	56.323	1.00	52.01	B
ATOM	224	OE2	GLU	42	51.883	-15.816	57.151	1.00	51.85	B
ATOM	225	C	GLU	42	47.050	-12.338	55.896	1.00	41.88	B
ATOM	226	O	GLU	42	46.193	-12.740	56.683	1.00	42.51	B
ATOM	227	N	CYS	43	46.754	-11.798	54.718	1.00	40.93	B
ATOM	228	CA	CYS	43	45.372	-11.670	54.275	1.00	41.17	B
ATOM	229	CB	CYS	43	45.102	-10.237	53.775	1.00	39.59	B
ATOM	230	SG	CYS	43	44.959	-9.008	55.115	1.00	41.44	B
ATOM	231	C	CYS	43	45.033	-12.682	53.185	1.00	42.27	B
ATOM	232	O	CYS	43	45.736	-12.781	52.182	1.00	43.23	B

ATOM	233	N	ASP	44	43.953	-13.435	53.394	1.00	43.10	B
ATOM	234	CA	ASP	44	43.504	-14.444	52.436	1.00	43.06	B
ATOM	235	CB	ASP	44	43.392	-15.831	53.138	1.00	45.99	B
ATOM	236	CG	ASP	44	43.414	-16.999	52.151	1.00	46.99	B
ATOM	237	OD1	ASP	44	42.678	-16.948	51.139	1.00	48.57	B
ATOM	238	OD2	ASP	44	44.167	-17.971	52.398	1.00	44.91	B
ATOM	239	C	ASP	44	42.140	-14.045	51.853	1.00	42.13	B
ATOM	240	O	ASP	44	41.093	-14.446	52.363	1.00	39.99	B
ATOM	241	N	PRO	45	42.142	-13.254	50.767	1.00	41.84	B
ATOM	242	CD	PRO	45	43.328	-12.853	49.990	1.00	40.65	B
ATOM	243	CA	PRO	45	40.917	-12.791	50.107	1.00	41.77	B
ATOM	244	CB	PRO	45	41.449	-12.001	48.918	1.00	41.50	B
ATOM	245	CG	PRO	45	42.755	-12.688	48.614	1.00	40.93	B
ATOM	246	C	PRO	45	39.940	-13.893	49.690	1.00	42.90	B
ATOM	247	O	PRO	45	38.750	-13.822	50.002	1.00	43.83	B
ATOM	248	N	VAL	46	40.429	-14.908	48.985	1.00	42.74	B
ATOM	249	CA	VAL	46	39.554	-15.990	48.552	1.00	42.50	B
ATOM	250	CB	VAL	46	40.348	-17.109	47.854	1.00	41.92	B
ATOM	251	CG1	VAL	46	39.428	-18.269	47.531	1.00	40.40	B
ATOM	252	CG2	VAL	46	40.983	-16.574	46.581	1.00	41.19	B
ATOM	253	C	VAL	46	38.813	-16.577	49.751	1.00	43.26	B
ATOM	254	O	VAL	46	37.587	-16.736	49.730	1.00	43.10	B
ATOM	255	N	ARG	47	39.563	-16.896	50.797	1.00	43.54	B
ATOM	256	CA	ARG	47	38.975	-17.455	52.007	1.00	44.21	B
ATOM	257	CB	ARG	47	40.031	-18.250	52.784	1.00	47.76	B
ATOM	258	CG	ARG	47	40.295	-19.635	52.203	1.00	52.08	B
ATOM	259	CD	ARG	47	41.776	-19.981	52.208	1.00	55.86	B
ATOM	260	NE	ARG	47	42.400	-19.743	53.508	1.00	59.28	B
ATOM	261	CZ	ARG	47	42.043	-20.346	54.638	1.00	60.15	B
ATOM	262	NH1	ARG	47	41.056	-21.237	54.639	1.00	60.50	B
ATOM	263	NH2	ARG	47	42.674	-20.051	55.770	1.00	60.66	B
ATOM	264	C	ARG	47	38.388	-16.360	52.883	1.00	41.71	B
ATOM	265	O	ARG	47	37.673	-16.643	53.845	1.00	40.72	B
ATOM	266	N	LYS	48	38.695	-15.112	52.537	1.00	39.92	B
ATOM	267	CA	LYS	48	38.205	-13.947	53.268	1.00	38.19	B
ATOM	268	CB	LYS	48	36.682	-13.912	53.223	1.00	38.15	B
ATOM	269	CG	LYS	48	36.106	-13.820	51.826	1.00	39.40	B
ATOM	270	CD	LYS	48	34.638	-14.236	51.809	1.00	39.31	B
ATOM	271	CE	LYS	48	34.020	-14.014	50.440	1.00	41.44	B
ATOM	272	NZ	LYS	48	34.853	-14.620	49.354	1.00	42.78	B
ATOM	273	C	LYS	48	38.670	-13.925	54.723	1.00	37.09	B
ATOM	274	O	LYS	48	37.905	-13.563	55.617	1.00	37.31	B
ATOM	275	N	GLU	49	39.917	-14.314	54.961	1.00	35.98	B
ATOM	276	CA	GLU	49	40.450	-14.327	56.315	1.00	36.33	B
ATOM	277	CB	GLU	49	40.861	-15.733	56.743	1.00	40.35	B
ATOM	278	CG	GLU	49	39.752	-16.767	56.761	1.00	46.19	B
ATOM	279	CD	GLU	49	40.261	-18.163	57.122	1.00	49.22	B
ATOM	280	OE1	GLU	49	39.482	-19.131	56.975	1.00	50.87	B
ATOM	281	OE2	GLU	49	41.431	-18.293	57.555	1.00	49.58	B
ATOM	282	C	GLU	49	41.669	-13.444	56.445	1.00	35.96	B
ATOM	283	O	GLU	49	42.326	-13.095	55.462	1.00	34.28	B
ATOM	284	N	VAL	50	41.967	-13.097	57.685	1.00	34.47	B
ATOM	285	CA	VAL	50	43.122	-12.292	57.999	1.00	34.53	B
ATOM	286	CB	VAL	50	42.704	-10.858	58.439	1.00	32.83	B
ATOM	287	CG1	VAL	50	41.653	-10.918	59.512	1.00	30.31	B
ATOM	288	CG2	VAL	50	43.916	-10.092	58.929	1.00	32.98	B
ATOM	289	C	VAL	50	43.782	-13.059	59.135	1.00	35.60	B
ATOM	290	O	VAL	50	43.136	-13.367	60.130	1.00	36.44	B
ATOM	291	N	SER	51	45.054	-13.411	58.976	1.00	36.72	B
ATOM	292	CA	SER	51	45.748	-14.157	60.022	1.00	36.92	B
ATOM	293	CB	SER	51	46.320	-15.481	59.447	1.00	37.59	B
ATOM	294	OG	SER	51	46.556	-16.427	60.482	1.00	36.23	B
ATOM	295	C	SER	51	46.857	-13.315	60.656	1.00	37.31	B
ATOM	296	O	SER	51	47.694	-12.731	59.960	1.00	36.32	B
ATOM	297	N	VAL	52	46.852	-13.265	61.984	1.00	37.74	B
ATOM	298	CA	VAL	52	47.817	-12.474	62.735	1.00	39.56	B
ATOM	299	CB	VAL	52	47.092	-11.558	63.749	1.00	38.44	B
ATOM	300	CG1	VAL	52	48.090	-10.668	64.454	1.00	37.83	B
ATOM	301	CG2	VAL	52	46.041	-10.737	63.042	1.00	37.78	B
ATOM	302	C	VAL	52	48.813	-13.328	63.507	1.00	41.45	B
ATOM	303	O	VAL	52	48.429	-14.296	64.167	1.00	41.94	B
ATOM	304	N	ARG	53	50.091	-12.968	63.434	1.00	43.18	B
ATOM	305	CA	ARG	53	51.106	-13.713	64.166	1.00	46.04	B

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ATOM    306  CB  ARG    53      52.452 -13.698  63.434  1.00 45.91      B
ATOM    307  CG  ARG    53      53.488 -14.619  64.064  1.00 44.72      B
ATOM    308  CD  ARG    53      54.490 -15.103  63.034  1.00 45.80      B
ATOM    309  NE  ARG    53      55.317 -14.018  62.514  1.00 46.75      B
ATOM    310  CZ  ARG    53      56.036 -14.095  61.398  1.00 45.30      B
ATOM    311  NH1 ARG    53      56.028 -15.209  60.675  1.00 44.24      B
ATOM    312  NH2 ARG    53      56.765 -13.056  61.011  1.00 44.19      B
ATOM    313  C   ARG    53      51.259 -13.092  65.540  1.00 47.93      B
ATOM    314  O   ARG    53      51.466 -11.884  65.667  1.00 48.40      B
ATOM    315  N   THR    54      51.156 -13.929  66.565  1.00 49.62      B
ATOM    316  CA  THR    54      51.257 -13.473  67.941  1.00 51.39      B
ATOM    317  CB  THR    54      49.941 -13.744  68.683  1.00 51.01      B
ATOM    318  OG1 THR    54      49.735 -15.157  68.795  1.00 49.13      B
ATOM    319  CG2 THR    54      48.775 -13.144  67.914  1.00 51.53      B
ATOM    320  C   THR    54      52.391 -14.139  68.709  1.00 52.60      B
ATOM    321  O   THR    54      52.439 -14.058  69.933  1.00 53.07      B
ATOM    322  N   GLY    55      53.309 -14.784  67.995  1.00 54.10      B
ATOM    323  CA  GLY    55      54.404 -15.459  68.666  1.00 57.08      B
ATOM    324  C   GLY    55      55.721 -15.519  67.914  1.00 59.62      B
ATOM    325  O   GLY    55      56.119 -14.549  67.264  1.00 59.27      B
ATOM    326  N   GLY    56      56.393 -16.668  68.016  1.00 60.97      B
ATOM    327  CA  GLY    56      57.682 -16.880  67.372  1.00 62.99      B
ATOM    328  C   GLY    56      57.782 -16.549  65.892  1.00 64.76      B
ATOM    329  O   GLY    56      56.940 -15.828  65.350  1.00 66.18      B
ATOM    330  N   LEU    57      58.818 -17.074  65.235  1.00 64.97      B
ATOM    331  CA  LEU    57      59.032 -16.821  63.809  1.00 64.92      B
ATOM    332  CB  LEU    57      60.508 -17.137  63.407  1.00 63.43      B
ATOM    333  CG  LEU    57      61.638 -16.508  64.258  1.00 63.25      B
ATOM    334  CD1 LEU    57      61.844 -17.335  65.520  1.00 62.77      B
ATOM    335  CD2 LEU    57      62.928 -16.452  63.459  1.00 61.76      B
ATOM    336  C   LEU    57      58.080 -17.654  62.951  1.00 65.79      B
ATOM    337  O   LEU    57      57.186 -18.328  63.470  1.00 65.88      B
ATOM    338  N   ALA    58      58.269 -17.597  61.636  1.00 65.65      B
ATOM    339  CA  ALA    58      57.435 -18.356  60.712  1.00 65.12      B
ATOM    340  CB  ALA    58      57.687 -17.891  59.286  1.00 65.82      B
ATOM    341  C   ALA    58      57.770 -19.838  60.847  1.00 64.20      B
ATOM    342  O   ALA    58      56.953 -20.709  60.525  1.00 64.59      B
ATOM    343  N   ASP    59      58.980 -20.099  61.340  1.00 62.61      B
ATOM    344  CA  ASP    59      59.509 -21.447  61.542  1.00 60.18      B
ATOM    345  CB  ASP    59      60.973 -21.335  62.035  1.00 60.66      B
ATOM    346  CG  ASP    59      61.622 -22.682  62.266  1.00 61.45      B
ATOM    347  OD1 ASP    59      61.396 -23.268  63.343  1.00 61.95      B
ATOM    348  OD2 ASP    59      62.356 -23.155  61.370  1.00 61.61      B
ATOM    349  C   ASP    59      58.663 -22.274  62.519  1.00 58.06      B
ATOM    350  O   ASP    59      58.519 -23.490  62.370  1.00 56.73      B
ATOM    351  N   LYS    60      58.109 -21.591  63.513  1.00 55.07      B
ATOM    352  CA  LYS    60      57.258 -22.200  64.528  1.00 52.63      B
ATOM    353  CB  LYS    60      58.107 -23.079  65.525  1.00 51.66      B
ATOM    354  CG  LYS    60      57.301 -23.696  66.672  1.00 51.86      B
ATOM    355  CD  LYS    60      58.046 -24.839  67.368  1.00 51.88      B
ATOM    356  CE  LYS    60      59.349 -24.373  68.011  1.00 53.18      B
ATOM    357  NZ  LYS    60      60.197 -25.492  68.528  1.00 52.09      B
ATOM    358  C   LYS    60      56.615 -21.023  65.248  1.00 51.19      B
ATOM    359  O   LYS    60      57.314 -20.124  65.724  1.00 51.41      B
ATOM    360  N   SER    61      55.287 -21.010  65.313  1.00 48.55      B
ATOM    361  CA  SER    61      54.599 -19.905  65.960  1.00 45.99      B
ATOM    362  CB  SER    61      54.881 -18.636  65.192  1.00 46.32      B
ATOM    363  OG  SER    61      54.559 -18.803  63.820  1.00 44.99      B
ATOM    364  C   SER    61      53.092 -20.082  66.086  1.00 45.35      B
ATOM    365  O   SER    61      52.491 -20.950  65.449  1.00 44.81      B
ATOM    366  N   SER    62      52.488 -19.242  66.922  1.00 43.72      B
ATOM    367  CA  SER    62      51.047 -19.261  67.131  1.00 41.95      B
ATOM    368  CB  SER    62      50.738 -19.050  68.592  1.00 41.39      B
ATOM    369  OG  SER    62      51.608 -18.079  69.135  1.00 41.34      B
ATOM    370  C   SER    62      50.440 -18.143  66.291  1.00 40.85      B
ATOM    371  O   SER    62      51.147 -17.229  65.872  1.00 39.19      B
ATOM    372  N   ARG    63      49.138 -18.221  66.031  1.00 40.24      B
ATOM    373  CA  ARG    63      48.461 -17.207  65.226  1.00 38.90      B
ATOM    374  CB  ARG    63      48.630 -17.514  63.695  1.00 39.76      B
ATOM    375  CG  ARG    63      50.074 -17.554  63.205  1.00 41.62      B
ATOM    376  CD  ARG    63      50.149 -17.897  61.725  1.00 43.20      B
ATOM    377  NE  ARG    63      49.763 -16.776  60.866  1.00 46.47      B
ATOM    378  CZ  ARG    63      50.526 -15.711  60.626  1.00 46.07      B
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ATOM	379	NH1	ARG	63	51.728	-15.613	61.178	1.00	47.55	B
ATOM	380	NH2	ARG	63	50.090	-14.741	59.833	1.00	45.86	B
ATOM	381	C	ARG	63	46.976	-17.131	65.558	1.00	37.75	B
ATOM	382	O	ARG	63	46.410	-18.050	66.143	1.00	36.32	B
ATOM	383	N	LYS	64	46.356	-16.019	65.174	1.00	37.15	B
ATOM	384	CA	LYS	64	44.931	-15.788	65.400	1.00	35.14	B
ATOM	385	CB	LYS	64	44.737	-14.607	66.342	1.00	36.48	B
ATOM	386	CG	LYS	64	45.236	-14.826	67.760	1.00	37.70	B
ATOM	387	CD	LYS	64	44.174	-15.510	68.604	1.00	40.04	B
ATOM	388	CE	LYS	64	44.488	-15.408	70.087	1.00	40.04	B
ATOM	389	NZ	LYS	64	43.325	-15.861	70.893	1.00	40.98	B
ATOM	390	C	LYS	64	44.316	-15.467	64.041	1.00	33.82	B
ATOM	391	O	LYS	64	44.811	-14.590	63.329	1.00	35.17	B
ATOM	392	N	THR	65	43.253	-16.173	63.669	1.00	31.23	B
ATOM	393	CA	THR	65	42.619	-15.928	62.377	1.00	30.10	B
ATOM	394	CB	THR	65	42.784	-17.141	61.438	1.00	32.25	B
ATOM	395	OG1	THR	65	44.171	-17.498	61.357	1.00	32.66	B
ATOM	396	CG2	THR	65	42.279	-16.799	60.028	1.00	33.40	B
ATOM	397	C	THR	65	41.133	-15.597	62.503	1.00	28.24	B
ATOM	398	O	THR	65	40.440	-16.116	63.382	1.00	28.59	B
ATOM	399	N	TYR	66	40.648	-14.720	61.630	1.00	24.28	B
ATOM	400	CA	TYR	66	39.244	-14.335	61.665	1.00	22.45	B
ATOM	401	CB	TYR	66	39.045	-12.976	62.362	1.00	19.03	B
ATOM	402	CG	TYR	66	39.783	-12.804	63.674	1.00	16.05	B
ATOM	403	CD1	TYR	66	41.158	-12.594	63.697	1.00	11.74	B
ATOM	404	CE1	TYR	66	41.829	-12.377	64.894	1.00	13.31	B
ATOM	405	CD2	TYR	66	39.094	-12.802	64.891	1.00	15.60	B
ATOM	406	CE2	TYR	66	39.753	-12.586	66.097	1.00	13.06	B
ATOM	407	CZ	TYR	66	41.121	-12.368	66.090	1.00	15.20	B
ATOM	408	OH	TYR	66	41.781	-12.100	67.272	1.00	19.72	B
ATOM	409	C	TYR	66	38.666	-14.241	60.271	1.00	22.39	B
ATOM	410	O	TYR	66	39.355	-13.876	59.317	1.00	21.02	B
ATOM	411	N	THR	67	37.387	-14.580	60.167	1.00	23.76	B
ATOM	412	CA	THR	67	36.678	-14.523	58.900	1.00	25.75	B
ATOM	413	CB	THR	67	35.789	-15.754	58.699	1.00	24.72	B
ATOM	414	OG1	THR	67	36.607	-16.923	58.702	1.00	28.23	B
ATOM	415	CG2	THR	67	35.043	-15.664	57.376	1.00	24.97	B
ATOM	416	C	THR	67	35.787	-13.291	58.864	1.00	26.39	B
ATOM	417	O	THR	67	35.036	-13.026	59.811	1.00	26.22	B
ATOM	418	N	PHE	68	35.899	-12.538	57.775	1.00	26.28	B
ATOM	419	CA	PHE	68	35.091	-11.342	57.565	1.00	27.23	B
ATOM	420	CB	PHE	68	35.942	-10.056	57.673	1.00	25.89	B
ATOM	421	CG	PHE	68	36.634	-9.893	58.997	1.00	27.52	B
ATOM	422	CD1	PHE	68	37.873	-10.485	59.230	1.00	26.70	B
ATOM	423	CD2	PHE	68	36.037	-9.161	60.023	1.00	26.12	B
ATOM	424	CE1	PHE	68	38.501	-10.350	60.464	1.00	25.62	B
ATOM	425	CE2	PHE	68	36.662	-9.025	61.258	1.00	25.03	B
ATOM	426	CZ	PHE	68	37.894	-9.619	61.478	1.00	25.92	B
ATOM	427	C	PHE	68	34.492	-11.434	56.171	1.00	27.19	B
ATOM	428	O	PHE	68	34.955	-12.206	55.328	1.00	27.43	B
ATOM	429	N	ASP	69	33.470	-10.631	55.926	1.00	26.71	B
ATOM	430	CA	ASP	69	32.805	-10.629	54.636	1.00	27.55	B
ATOM	431	CB	ASP	69	31.660	-9.635	54.684	1.00	27.61	B
ATOM	432	CG	ASP	69	30.623	-10.019	55.735	1.00	28.58	B
ATOM	433	OD1	ASP	69	30.578	-9.403	56.831	1.00	27.66	B
ATOM	434	OD2	ASP	69	29.865	-10.972	55.461	1.00	28.48	B
ATOM	435	C	ASP	69	33.738	-10.366	53.458	1.00	27.41	B
ATOM	436	O	ASP	69	33.455	-10.771	52.334	1.00	27.23	B
ATOM	437	N	MET	70	34.861	-9.710	53.732	1.00	28.30	B
ATOM	438	CA	MET	70	35.865	-9.396	52.717	1.00	28.88	B
ATOM	439	CB	MET	70	35.424	-8.213	51.821	1.00	30.69	B
ATOM	440	CG	MET	70	34.283	-8.469	50.867	1.00	31.73	B
ATOM	441	SD	MET	70	33.894	-6.957	49.923	1.00	36.68	B
ATOM	442	CE	MET	70	32.083	-7.049	49.877	1.00	34.73	B
ATOM	443	C	MET	70	37.141	-8.983	53.433	1.00	28.83	B
ATOM	444	O	MET	70	37.098	-8.480	54.553	1.00	29.82	B
ATOM	445	N	VAL	71	38.274	-9.188	52.780	1.00	27.33	B
ATOM	446	CA	VAL	71	39.553	-8.812	53.349	1.00	26.23	B
ATOM	447	CB	VAL	71	40.291	-10.021	54.003	1.00	27.99	B
ATOM	448	CG1	VAL	71	39.635	-10.381	55.319	1.00	28.32	B
ATOM	449	CG2	VAL	71	40.264	-11.219	53.076	1.00	28.60	B
ATOM	450	C	VAL	71	40.398	-8.233	52.231	1.00	25.01	B
ATOM	451	O	VAL	71	40.363	-8.713	51.100	1.00	24.55	B

ATOM	452	N	PHE	72	41.146	-7.191	52.571	1.00	24.93	B
ATOM	453	CA	PHE	72	42.005	-6.475	51.645	1.00	24.43	B
ATOM	454	CB	PHE	72	41.444	-5.076	51.392	1.00	23.95	B
ATOM	455	CG	PHE	72	40.024	-5.059	50.903	1.00	23.17	B
ATOM	456	CD1	PHE	72	39.722	-5.376	49.583	1.00	22.75	B
ATOM	457	CD2	PHE	72	38.991	-4.680	51.754	1.00	23.31	B
ATOM	458	CE1	PHE	72	38.414	-5.310	49.113	1.00	23.87	B
ATOM	459	CE2	PHE	72	37.679	-4.612	51.294	1.00	23.71	B
ATOM	460	CZ	PHE	72	37.389	-4.927	49.970	1.00	24.15	B
ATOM	461	C	PHE	72	43.381	-6.321	52.266	1.00	25.11	B
ATOM	462	O	PHE	72	43.522	-5.683	53.312	1.00	26.80	B
ATOM	463	N	GLY	73	44.394	-6.885	51.621	1.00	24.77	B
ATOM	464	CA	GLY	73	45.741	-6.774	52.142	1.00	23.03	B
ATOM	465	C	GLY	73	46.352	-5.450	51.743	1.00	26.33	B
ATOM	466	O	GLY	73	45.698	-4.594	51.141	1.00	26.76	B
ATOM	467	N	ALA	74	47.626	-5.284	52.062	1.00	27.88	B
ATOM	468	CA	ALA	74	48.335	-4.054	51.752	1.00	28.98	B
ATOM	469	CB	ALA	74	49.690	-4.074	52.427	1.00	29.52	B
ATOM	470	C	ALA	74	48.505	-3.802	50.260	1.00	29.91	B
ATOM	471	O	ALA	74	49.037	-2.773	49.865	1.00	31.84	B
ATOM	472	N	SER	75	48.051	-4.726	49.426	1.00	31.43	B
ATOM	473	CA	SER	75	48.209	-4.558	47.982	1.00	34.31	B
ATOM	474	CB	SER	75	48.382	-5.914	47.318	1.00	32.52	B
ATOM	475	OG	SER	75	49.088	-6.785	48.183	1.00	36.15	B
ATOM	476	C	SER	75	46.994	-3.858	47.395	1.00	34.29	B
ATOM	477	O	SER	75	47.066	-3.236	46.327	1.00	34.53	B
ATOM	478	N	THR	76	45.882	-3.963	48.111	1.00	32.69	B
ATOM	479	CA	THR	76	44.635	-3.364	47.675	1.00	32.77	B
ATOM	480	CB	THR	76	43.530	-3.549	48.744	1.00	32.84	B
ATOM	481	OG1	THR	76	43.612	-4.863	49.305	1.00	31.95	B
ATOM	482	CG2	THR	76	42.158	-3.380	48.120	1.00	33.21	B
ATOM	483	C	THR	76	44.803	-1.870	47.403	1.00	31.46	B
ATOM	484	O	THR	76	45.305	-1.134	48.251	1.00	32.33	B
ATOM	485	N	LYS	77	44.394	-1.430	46.218	1.00	29.15	B
ATOM	486	CA	LYS	77	44.469	-0.015	45.875	1.00	27.33	B
ATOM	487	CB	LYS	77	44.906	0.155	44.423	1.00	29.39	B
ATOM	488	CG	LYS	77	46.342	-0.341	44.187	1.00	32.84	B
ATOM	489	CD	LYS	77	46.949	0.180	42.884	1.00	36.59	B
ATOM	490	CE	LYS	77	46.241	-0.349	41.627	1.00	38.03	B
ATOM	491	NZ	LYS	77	44.818	0.106	41.501	1.00	38.31	B
ATOM	492	C	LYS	77	43.096	0.625	46.134	1.00	25.52	B
ATOM	493	O	LYS	77	42.127	-0.088	46.371	1.00	23.25	B
ATOM	494	N	GLN	78	43.018	1.956	46.115	1.00	24.22	B
ATOM	495	CA	GLN	78	41.759	2.652	46.398	1.00	22.43	B
ATOM	496	CB	GLN	78	41.935	4.177	46.226	1.00	22.53	B
ATOM	497	CG	GLN	78	43.014	4.799	47.088	1.00	21.23	B
ATOM	498	CD	GLN	78	42.603	4.953	48.539	1.00	20.15	B
ATOM	499	OE1	GLN	78	42.235	3.988	49.192	1.00	18.03	B
ATOM	500	NE2	GLN	78	42.661	6.178	49.045	1.00	21.65	B
ATOM	501	C	GLN	78	40.624	2.177	45.504	1.00	22.10	B
ATOM	502	O	GLN	78	39.533	1.839	45.986	1.00	20.46	B
ATOM	503	N	ILE	79	40.898	2.153	44.203	1.00	21.56	B
ATOM	504	CA	ILE	79	39.929	1.746	43.194	1.00	23.67	B
ATOM	505	CB	ILE	79	40.590	1.749	41.774	1.00	23.18	B
ATOM	506	CG2	ILE	79	41.716	0.732	41.715	1.00	24.28	B
ATOM	507	CG1	ILE	79	39.574	1.416	40.705	1.00	21.98	B
ATOM	508	CD1	ILE	79	38.563	2.492	40.470	1.00	23.15	B
ATOM	509	C	ILE	79	39.303	0.366	43.475	1.00	25.91	B
ATOM	510	O	ILE	79	38.142	0.120	43.122	1.00	26.57	B
ATOM	511	N	ASP	80	40.061	-0.527	44.107	1.00	24.45	B
ATOM	512	CA	ASP	80	39.547	-1.857	44.416	1.00	25.05	B
ATOM	513	CB	ASP	80	40.694	-2.832	44.721	1.00	25.59	B
ATOM	514	CG	ASP	80	41.691	-2.928	43.588	1.00	26.46	B
ATOM	515	OD1	ASP	80	41.248	-2.925	42.414	1.00	26.20	B
ATOM	516	OD2	ASP	80	42.912	-3.016	43.877	1.00	27.35	B
ATOM	517	C	ASP	80	38.612	-1.809	45.611	1.00	24.84	B
ATOM	518	O	ASP	80	37.638	-2.553	45.686	1.00	23.83	B
ATOM	519	N	VAL	81	38.924	-0.934	46.556	1.00	25.12	B
ATOM	520	CA	VAL	81	38.102	-0.794	47.742	1.00	25.00	B
ATOM	521	CB	VAL	81	38.749	0.174	48.750	1.00	22.43	B
ATOM	522	CG1	VAL	81	37.698	0.713	49.716	1.00	21.58	B
ATOM	523	CG2	VAL	81	39.855	-0.555	49.509	1.00	20.63	B
ATOM	524	C	VAL	81	36.753	-0.250	47.320	1.00	27.16	B

ATOM	525	O	VAL	81	35.707	-0.746	47.747	1.00	27.22	B
ATOM	526	N	TYR	82	36.792	0.769	46.464	1.00	27.98	B
ATOM	527	CA	TYR	82	35.580	1.406	45.987	1.00	28.04	B
ATOM	528	CB	TYR	82	35.922	2.661	45.125	1.00	27.34	B
ATOM	529	CG	TYR	82	34.681	3.366	44.637	1.00	26.71	B
ATOM	530	CD1	TYR	82	34.262	3.252	43.315	1.00	26.63	B
ATOM	531	CE1	TYR	82	33.054	3.808	42.893	1.00	29.11	B
ATOM	532	CD2	TYR	82	33.866	4.063	45.529	1.00	27.27	B
ATOM	533	CE2	TYR	82	32.660	4.620	45.128	1.00	28.67	B
ATOM	534	CZ	TYR	82	32.257	4.488	43.809	1.00	30.95	B
ATOM	535	OH	TYR	82	31.047	5.021	43.418	1.00	34.58	B
ATOM	536	C	TYR	82	34.705	0.454	45.183	1.00	29.38	B
ATOM	537	O	TYR	82	33.498	0.322	45.448	1.00	28.44	B
ATOM	538	N	ARG	83	35.312	-0.212	44.206	1.00	30.12	B
ATOM	539	CA	ARG	83	34.569	-1.136	43.365	1.00	32.33	B
ATOM	540	CB	ARG	83	35.475	-1.667	42.238	1.00	32.84	B
ATOM	541	CG	ARG	83	35.814	-0.610	41.177	1.00	36.78	B
ATOM	542	CD	ARG	83	36.995	-1.024	40.298	1.00	39.59	B
ATOM	543	NE	ARG	83	36.692	-2.180	39.459	1.00	45.16	B
ATOM	544	CZ	ARG	83	36.158	-2.110	38.242	1.00	46.77	B
ATOM	545	NH1	ARG	83	35.870	-0.930	37.706	1.00	47.42	B
ATOM	546	NH2	ARG	83	35.897	-3.226	37.567	1.00	47.17	B
ATOM	547	C	ARG	83	33.930	-2.291	44.142	1.00	32.86	B
ATOM	548	O	ARG	83	32.786	-2.658	43.866	1.00	34.02	B
ATOM	549	N	SER	84	34.648	-2.834	45.125	1.00	32.13	B
ATOM	550	CA	SER	84	34.159	-3.959	45.933	1.00	30.95	B
ATOM	551	CB	SER	84	35.347	-4.712	46.558	1.00	32.34	B
ATOM	552	OG	SER	84	36.301	-5.060	45.568	1.00	37.12	B
ATOM	553	C	SER	84	33.186	-3.593	47.046	1.00	29.09	B
ATOM	554	O	SER	84	32.151	-4.241	47.225	1.00	29.03	B
ATOM	555	N	VAL	85	33.522	-2.570	47.815	1.00	27.74	B
ATOM	556	CA	VAL	85	32.652	-2.176	48.911	1.00	27.01	B
ATOM	557	CB	VAL	85	33.481	-1.800	50.165	1.00	25.48	B
ATOM	558	CG1	VAL	85	32.566	-1.623	51.354	1.00	24.98	B
ATOM	559	CG2	VAL	85	34.514	-2.865	50.448	1.00	26.13	B
ATOM	560	C	VAL	85	31.684	-1.024	48.613	1.00	25.90	B
ATOM	561	O	VAL	85	30.480	-1.167	48.779	1.00	24.94	B
ATOM	562	N	VAL	86	32.205	0.106	48.152	1.00	26.94	B
ATOM	563	CA	VAL	86	31.368	1.281	47.916	1.00	27.62	B
ATOM	564	CB	VAL	86	32.227	2.551	47.793	1.00	25.49	B
ATOM	565	CG1	VAL	86	31.384	3.763	48.096	1.00	25.95	B
ATOM	566	CG2	VAL	86	33.418	2.480	48.722	1.00	24.40	B
ATOM	567	C	VAL	86	30.395	1.267	46.736	1.00	28.91	B
ATOM	568	O	VAL	86	29.254	1.709	46.874	1.00	27.52	B
ATOM	569	N	CYS	87	30.835	0.773	45.583	1.00	30.20	B
ATOM	570	CA	CYS	87	29.978	0.748	44.402	1.00	31.96	B
ATOM	571	CB	CYS	87	30.692	0.026	43.257	1.00	35.17	B
ATOM	572	SG	CYS	87	30.072	0.418	41.599	1.00	41.71	B
ATOM	573	C	CYS	87	28.593	0.126	44.653	1.00	32.37	B
ATOM	574	O	CYS	87	27.571	0.682	44.234	1.00	31.48	B
ATOM	575	N	PRO	88	28.538	-1.028	45.347	1.00	31.98	B
ATOM	576	CD	PRO	88	29.675	-1.840	45.803	1.00	32.51	B
ATOM	577	CA	PRO	88	27.272	-1.712	45.648	1.00	30.72	B
ATOM	578	CB	PRO	88	27.720	-3.024	46.269	1.00	31.27	B
ATOM	579	CG	PRO	88	29.104	-3.223	45.739	1.00	32.03	B
ATOM	580	C	PRO	88	26.407	-0.907	46.617	1.00	30.37	B
ATOM	581	O	PRO	88	25.179	-0.928	46.528	1.00	29.46	B
ATOM	582	N	ILE	89	27.060	-0.214	47.549	1.00	28.89	B
ATOM	583	CA	ILE	89	26.372	0.607	48.539	1.00	26.92	B
ATOM	584	CB	ILE	89	27.325	1.032	49.677	1.00	27.36	B
ATOM	585	CG2	ILE	89	26.562	1.827	50.728	1.00	29.65	B
ATOM	586	CG1	ILE	89	27.949	-0.202	50.327	1.00	28.47	B
ATOM	587	CD1	ILE	89	28.880	0.116	51.493	1.00	28.07	B
ATOM	588	C	ILE	89	25.815	1.866	47.883	1.00	26.45	B
ATOM	589	O	ILE	89	24.733	2.329	48.236	1.00	25.57	B
ATOM	590	N	LEU	90	26.551	2.416	46.922	1.00	26.88	B
ATOM	591	CA	LEU	90	26.097	3.618	46.242	1.00	27.21	B
ATOM	592	CB	LEU	90	27.185	4.167	45.305	1.00	26.30	B
ATOM	593	CG	LEU	90	26.768	5.457	44.531	1.00	28.27	B
ATOM	594	CD1	LEU	90	26.300	6.546	45.499	1.00	27.39	B
ATOM	595	CD2	LEU	90	27.936	5.952	43.707	1.00	30.13	B
ATOM	596	C	LEU	90	24.828	3.334	45.451	1.00	28.12	B
ATOM	597	O	LEU	90	23.914	4.156	45.423	1.00	27.80	B

ATOM	598	N	ASP	91	24.778	2.168	44.811	1.00	29.04	B
ATOM	599	CA	ASP	91	23.615	1.782	44.029	1.00	29.68	B
ATOM	600	CB	ASP	91	23.888	0.479	43.238	1.00	30.25	B
ATOM	601	CG	ASP	91	24.715	0.717	41.975	1.00	33.21	B
ATOM	602	OD1	ASP	91	24.655	1.836	41.417	1.00	33.99	B
ATOM	603	OD2	ASP	91	25.409	-0.225	41.522	1.00	34.57	B
ATOM	604	C	ASP	91	22.412	1.604	44.950	1.00	29.79	B
ATOM	605	O	ASP	91	21.265	1.785	44.542	1.00	29.34	B
ATOM	606	N	GLU	92	22.684	1.254	46.199	1.00	30.26	B
ATOM	607	CA	GLU	92	21.632	1.077	47.191	1.00	33.20	B
ATOM	608	CB	GLU	92	22.240	0.434	48.455	1.00	37.58	B
ATOM	609	CG	GLU	92	21.243	-0.021	49.519	1.00	45.34	B
ATOM	610	CD	GLU	92	20.622	-1.378	49.215	1.00	49.33	B
ATOM	611	OE1	GLU	92	19.996	-1.963	50.134	1.00	51.49	B
ATOM	612	OE2	GLU	92	20.760	-1.851	48.061	1.00	50.48	B
ATOM	613	C	GLU	92	21.036	2.471	47.516	1.00	32.34	B
ATOM	614	O	GLU	92	19.816	2.659	47.548	1.00	31.40	B
ATOM	615	N	VAL	93	21.921	3.438	47.757	1.00	29.83	B
ATOM	616	CA	VAL	93	21.532	4.813	48.060	1.00	27.09	B
ATOM	617	CB	VAL	93	22.794	5.732	48.216	1.00	27.00	B
ATOM	618	CG1	VAL	93	22.362	7.185	48.503	1.00	23.70	B
ATOM	619	CG2	VAL	93	23.720	5.189	49.320	1.00	24.02	B
ATOM	620	C	VAL	93	20.661	5.384	46.936	1.00	25.06	B
ATOM	621	O	VAL	93	19.631	6.005	47.184	1.00	23.16	B
ATOM	622	N	ILE	94	21.090	5.173	45.700	1.00	23.81	B
ATOM	623	CA	ILE	94	20.357	5.679	44.554	1.00	26.20	B
ATOM	624	CB	ILE	94	21.196	5.496	43.268	1.00	24.09	B
ATOM	625	CG2	ILE	94	20.398	5.871	42.040	1.00	22.58	B
ATOM	626	CG1	ILE	94	22.436	6.394	43.367	1.00	23.30	B
ATOM	627	CD1	ILE	94	23.378	6.288	42.211	1.00	25.19	B
ATOM	628	C	ILE	94	18.964	5.057	44.417	1.00	28.52	B
ATOM	629	O	ILE	94	18.101	5.606	43.742	1.00	30.41	B
ATOM	630	N	MET	95	18.729	3.925	45.073	1.00	31.00	B
ATOM	631	CA	MET	95	17.408	3.305	45.032	1.00	32.10	B
ATOM	632	CB	MET	95	17.501	1.789	45.171	1.00	35.87	B
ATOM	633	CG	MET	95	17.836	1.059	43.885	1.00	39.09	B
ATOM	634	SD	MET	95	17.725	-0.743	44.078	1.00	46.44	B
ATOM	635	CE	MET	95	19.451	-1.155	44.567	1.00	42.73	B
ATOM	636	C	MET	95	16.514	3.857	46.140	1.00	31.79	B
ATOM	637	O	MET	95	15.340	3.518	46.204	1.00	32.44	B
ATOM	638	N	GLY	96	17.069	4.697	47.016	1.00	31.15	B
ATOM	639	CA	GLY	96	16.274	5.290	48.083	1.00	30.86	B
ATOM	640	C	GLY	96	16.506	4.778	49.497	1.00	31.33	B
ATOM	641	O	GLY	96	15.695	5.005	50.398	1.00	31.96	B
ATOM	642	N	TYR	97	17.617	4.085	49.700	1.00	31.69	B
ATOM	643	CA	TYR	97	17.951	3.539	51.009	1.00	31.47	B
ATOM	644	CB	TYR	97	18.620	2.119	50.859	1.00	35.21	B
ATOM	645	CG	TYR	97	17.707	0.979	50.448	1.00	38.09	B
ATOM	646	CD1	TYR	97	16.856	0.369	51.374	1.00	38.78	B
ATOM	647	CE1	TYR	97	16.060	-0.716	51.017	1.00	39.92	B
ATOM	648	CD2	TYR	97	17.733	0.476	49.146	1.00	38.17	B
ATOM	649	CE2	TYR	97	16.938	-0.606	48.777	1.00	40.59	B
ATOM	650	CZ	TYR	97	16.105	-1.197	49.717	1.00	42.01	B
ATOM	651	OH	TYR	97	15.314	-2.262	49.350	1.00	44.26	B
ATOM	652	C	TYR	97	18.944	4.465	51.699	1.00	29.27	B
ATOM	653	O	TYR	97	19.557	5.309	51.055	1.00	29.87	B
ATOM	654	N	ASN	98	19.089	4.308	53.008	1.00	26.93	B
ATOM	655	CA	ASN	98	20.061	5.081	53.768	1.00	27.11	B
ATOM	656	CB	ASN	98	19.500	5.509	55.156	1.00	27.12	B
ATOM	657	CG	ASN	98	18.435	6.579	55.048	1.00	27.28	B
ATOM	658	OD1	ASN	98	18.553	7.506	54.245	1.00	30.11	B
ATOM	659	ND2	ASN	98	17.394	6.465	55.860	1.00	26.60	B
ATOM	660	C	ASN	98	21.243	4.141	53.975	1.00	26.22	B
ATOM	661	O	ASN	98	21.055	2.971	54.292	1.00	25.58	B
ATOM	662	N	CYS	99	22.457	4.634	53.775	1.00	25.47	B
ATOM	663	CA	CYS	99	23.629	3.791	53.977	1.00	25.10	B
ATOM	664	CB	CYS	99	24.206	3.357	52.654	1.00	26.81	B
ATOM	665	SG	CYS	99	23.084	2.317	51.714	1.00	26.81	B
ATOM	666	C	CYS	99	24.697	4.486	54.798	1.00	23.75	B
ATOM	667	O	CYS	99	24.804	5.712	54.804	1.00	25.67	B
ATOM	668	N	THR	100	25.482	3.683	55.496	1.00	20.94	B
ATOM	669	CA	THR	100	26.549	4.181	56.341	1.00	19.27	B
ATOM	670	CB	THR	100	26.076	4.266	57.795	1.00	17.86	B

ATOM	671	OG1	THR	100	24.992	5.192	57.875	1.00	16.90	B
ATOM	672	CG2	THR	100	27.202	4.714	58.708	1.00	17.10	B
ATOM	673	C	THR	100	27.760	3.247	56.269	1.00	19.78	B
ATOM	674	O	THR	100	27.615	2.013	56.297	1.00	19.41	B
ATOM	675	N	ILE	101	28.945	3.846	56.170	1.00	17.12	B
ATOM	676	CA	ILE	101	30.194	3.096	56.112	1.00	13.84	B
ATOM	677	CB	ILE	101	30.923	3.273	54.770	1.00	11.63	B
ATOM	678	CG2	ILE	101	32.193	2.459	54.763	1.00	11.54	B
ATOM	679	CG1	ILE	101	30.029	2.847	53.614	1.00	11.12	B
ATOM	680	CD1	ILE	101	30.610	3.205	52.240	1.00	8.60	B
ATOM	681	C	ILE	101	31.088	3.655	57.189	1.00	14.61	B
ATOM	682	O	ILE	101	31.434	4.828	57.158	1.00	16.06	B
ATOM	683	N	PHE	102	31.454	2.814	58.149	1.00	16.69	B
ATOM	684	CA	PHE	102	32.336	3.214	59.246	1.00	15.45	B
ATOM	685	CB	PHE	102	31.957	2.509	60.517	1.00	15.38	B
ATOM	686	CG	PHE	102	30.704	3.002	61.158	1.00	17.02	B
ATOM	687	CD1	PHE	102	30.746	4.068	62.060	1.00	14.70	B
ATOM	688	CD2	PHE	102	29.489	2.341	60.937	1.00	15.06	B
ATOM	689	CE1	PHE	102	29.601	4.468	62.744	1.00	15.17	B
ATOM	690	CE2	PHE	102	28.336	2.732	61.614	1.00	16.46	B
ATOM	691	CZ	PHE	102	28.389	3.797	62.523	1.00	16.06	B
ATOM	692	C	PHE	102	33.770	2.789	58.956	1.00	13.66	B
ATOM	693	O	PHE	102	34.004	1.767	58.335	1.00	14.29	B
ATOM	694	N	ALA	103	34.723	3.571	59.431	1.00	14.00	B
ATOM	695	CA	ALA	103	36.135	3.230	59.309	1.00	13.68	B
ATOM	696	CB	ALA	103	36.894	4.316	58.595	1.00	12.73	B
ATOM	697	C	ALA	103	36.579	3.142	60.771	1.00	14.68	B
ATOM	698	O	ALA	103	36.560	4.144	61.491	1.00	12.81	B
ATOM	699	N	TYR	104	36.943	1.939	61.211	1.00	14.23	B
ATOM	700	CA	TYR	104	37.369	1.722	62.588	1.00	13.28	B
ATOM	701	CB	TYR	104	36.415	0.741	63.271	1.00	13.08	B
ATOM	702	CG	TYR	104	36.704	0.496	64.740	1.00	9.23	B
ATOM	703	CD1	TYR	104	37.774	-0.304	65.139	1.00	10.77	B
ATOM	704	CE1	TYR	104	38.050	-0.519	66.497	1.00	8.87	B
ATOM	705	CD2	TYR	104	35.916	1.072	65.728	1.00	7.28	B
ATOM	706	CE2	TYR	104	36.180	0.861	67.085	1.00	6.26	B
ATOM	707	CZ	TYR	104	37.245	0.063	67.459	1.00	6.63	B
ATOM	708	OH	TYR	104	37.492	-0.189	68.791	1.00	6.91	B
ATOM	709	C	TYR	104	38.791	1.191	62.660	1.00	14.55	B
ATOM	710	O	TYR	104	39.192	0.344	61.866	1.00	17.36	B
ATOM	711	N	GLY	105	39.553	1.688	63.622	1.00	15.00	B
ATOM	712	CA	GLY	105	40.920	1.239	63.760	1.00	16.15	B
ATOM	713	C	GLY	105	41.818	2.222	64.480	1.00	18.48	B
ATOM	714	O	GLY	105	41.464	3.383	64.733	1.00	19.06	B
ATOM	715	N	GLN	106	42.996	1.726	64.818	1.00	18.69	B
ATOM	716	CA	GLN	106	44.012	2.480	65.524	1.00	20.40	B
ATOM	717	CB	GLN	106	45.109	1.510	65.958	1.00	20.92	B
ATOM	718	CG	GLN	106	46.494	2.093	65.959	1.00	25.11	B
ATOM	719	CD	GLN	106	47.546	1.104	66.424	1.00	27.12	B
ATOM	720	OE1	GLN	106	47.724	0.033	65.833	1.00	29.47	B
ATOM	721	NE2	GLN	106	48.254	1.462	67.486	1.00	24.05	B
ATOM	722	C	GLN	106	44.595	3.602	64.668	1.00	22.74	B
ATOM	723	O	GLN	106	44.733	3.442	63.447	1.00	22.56	B
ATOM	724	N	THR	107	44.924	4.733	65.312	1.00	22.64	B
ATOM	725	CA	THR	107	45.526	5.893	64.637	1.00	21.79	B
ATOM	726	CB	THR	107	46.070	6.943	65.659	1.00	22.17	B
ATOM	727	OG1	THR	107	45.014	7.404	66.510	1.00	22.36	B
ATOM	728	CG2	THR	107	46.675	8.142	64.927	1.00	19.97	B
ATOM	729	C	THR	107	46.720	5.430	63.788	1.00	21.90	B
ATOM	730	O	THR	107	47.605	4.752	64.288	1.00	20.99	B
ATOM	731	N	GLY	108	46.739	5.796	62.510	1.00	22.46	B
ATOM	732	CA	GLY	108	47.836	5.394	61.652	1.00	21.62	B
ATOM	733	C	GLY	108	47.664	4.088	60.882	1.00	22.90	B
ATOM	734	O	GLY	108	48.653	3.547	60.376	1.00	24.07	B
ATOM	735	N	THR	109	46.436	3.572	60.786	1.00	22.29	B
ATOM	736	CA	THR	109	46.197	2.321	60.050	1.00	21.18	B
ATOM	737	CB	THR	109	45.408	1.259	60.884	1.00	21.26	B
ATOM	738	OG1	THR	109	44.159	1.814	61.335	1.00	20.11	B
ATOM	739	CG2	THR	109	46.250	0.777	62.071	1.00	19.60	B
ATOM	740	C	THR	109	45.439	2.523	58.754	1.00	19.58	B
ATOM	741	O	THR	109	45.126	1.551	58.068	1.00	20.97	B
ATOM	742	N	GLY	110	45.125	3.776	58.428	1.00	17.22	B
ATOM	743	CA	GLY	110	44.415	4.048	57.193	1.00	12.69	B

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ATOM    744  C   GLY   110      42.943   4.424  57.232  1.00 12.29      B
ATOM    745  O   GLY   110      42.288   4.365  56.193  1.00 14.37      B
ATOM    746  N   LYS   111      42.398   4.795  58.386  1.00 11.41      B
ATOM    747  CA  LYS   111      40.983   5.198  58.432  1.00 12.47      B
ATOM    748  CB  LYS   111      40.540   5.653  59.898  1.00 13.24      B
ATOM    749  CG  LYS   111      40.379   4.538  60.934  1.00 10.82      B
ATOM    750  CD  LYS   111      39.805   5.061  62.229  1.00  6.09      B
ATOM    751  CE  LYS   111      40.691   6.142  62.813  1.00 10.33      B
ATOM    752  NZ  LYS   111      42.130   5.748  63.038  1.00  9.60      B
ATOM    753  C   LYS   111      40.742   6.363  57.465  1.00 13.44      B
ATOM    754  O   LYS   111      39.870   6.295  56.587  1.00 14.48      B
ATOM    755  N   THR   112      41.538   7.423  57.614  1.00 14.82      B
ATOM    756  CA  THR   112      41.403   8.613  56.773  1.00 15.93      B
ATOM    757  CB  THR   112      42.140   9.793  57.417  1.00 15.93      B
ATOM    758  OG1 THR   112      41.538  10.066  58.694  1.00 14.63      B
ATOM    759  CG2 THR   112      42.055  11.040  56.522  1.00 13.41      B
ATOM    760  C   THR   112      41.870   8.426  55.323  1.00 17.21      B
ATOM    761  O   THR   112      41.318   9.021  54.385  1.00 16.82      B
ATOM    762  N   PHE   113      42.887   7.595  55.142  1.00 17.40      B
ATOM    763  CA  PHE   113      43.398   7.313  53.811  1.00 16.82      B
ATOM    764  CB  PHE   113      44.654   6.389  53.889  1.00 16.02      B
ATOM    765  CG  PHE   113      45.233   6.054  52.540  1.00 17.10      B
ATOM    766  CD1 PHE   113      46.126   6.918  51.920  1.00 18.15      B
ATOM    767  CD2 PHE   113      44.836   4.911  51.868  1.00 18.15      B
ATOM    768  CE1 PHE   113      46.614   6.654  50.652  1.00 19.37      B
ATOM    769  CE2 PHE   113      45.317   4.632  50.588  1.00 20.77      B
ATOM    770  CZ  PHE   113      46.208   5.508  49.980  1.00 21.58      B
ATOM    771  C   PHE   113      42.305   6.615  52.997  1.00 15.35      B
ATOM    772  O   PHE   113      42.125   6.894  51.816  1.00 13.50      B
ATOM    773  N   THR   114      41.590   5.700  53.647  1.00 14.49      B
ATOM    774  CA  THR   114      40.524   4.942  53.008  1.00 13.72      B
ATOM    775  CB  THR   114      40.119   3.722  53.868  1.00 14.47      B
ATOM    776  OG1 THR   114      41.228   2.834  53.980  1.00 13.50      B
ATOM    777  CG2 THR   114      38.944   2.984  53.258  1.00 10.99      B
ATOM    778  C   THR   114      39.283   5.773  52.764  1.00 13.62      B
ATOM    779  O   THR   114      38.733   5.758  51.674  1.00 14.61      B
ATOM    780  N   MET   115      38.842   6.499  53.784  1.00 15.54      B
ATOM    781  CA  MET   115      37.635   7.311  53.663  1.00 16.98      B
ATOM    782  CB  MET   115      37.121   7.711  55.043  1.00 17.73      B
ATOM    783  CG  MET   115      36.776   6.525  55.938  1.00 22.32      B
ATOM    784  SD  MET   115      35.694   5.280  55.139  1.00 24.33      B
ATOM    785  CE  MET   115      34.110   6.102  55.162  1.00 17.96      B
ATOM    786  C   MET   115      37.772   8.556  52.809  1.00 16.94      B
ATOM    787  O   MET   115      36.824   8.956  52.140  1.00 17.35      B
ATOM    788  N   GLU   116      38.947   9.168  52.816  1.00 16.96      B
ATOM    789  CA  GLU   116      39.139  10.391  52.040  1.00 17.40      B
ATOM    790  CB  GLU   116      39.564  11.563  52.988  1.00 17.75      B
ATOM    791  CG  GLU   116      38.457  12.038  53.929  1.00 20.71      B
ATOM    792  CD  GLU   116      38.980  12.893  55.070  1.00 22.10      B
ATOM    793  OE1 GLU   116      40.113  13.404  54.961  1.00 26.78      B
ATOM    794  OE2 GLU   116      38.260  13.064  56.074  1.00 22.44      B
ATOM    795  C   GLU   116      40.178  10.211  50.953  1.00 16.14      B
ATOM    796  O   GLU   116      39.925  10.474  49.783  1.00 12.66      B
ATOM    797  N   GLY   117      41.357   9.768  51.360  1.00 16.93      B
ATOM    798  CA  GLY   117      42.425   9.585  50.406  1.00 21.10      B
ATOM    799  C   GLY   117      43.424  10.723  50.439  1.00 22.08      B
ATOM    800  O   GLY   117      43.321  11.640  51.248  1.00 21.52      B
ATOM    801  N   GLU   118      44.390  10.661  49.536  1.00 24.00      B
ATOM    802  CA  GLU   118      45.436  11.664  49.457  1.00 26.12      B
ATOM    803  CB  GLU   118      46.712  11.116  50.134  1.00 27.39      B
ATOM    804  CG  GLU   118      46.574  11.023  51.647  1.00 32.78      B
ATOM    805  CD  GLU   118      47.603  10.111  52.316  1.00 37.03      B
ATOM    806  OE1 GLU   118      48.799  10.149  51.938  1.00 36.38      B
ATOM    807  OE2 GLU   118      47.208   9.369  53.246  1.00 39.57      B
ATOM    808  C   GLU   118      45.702  12.026  48.000  1.00 26.11      B
ATOM    809  O   GLU   118      45.079  11.481  47.088  1.00 24.83      B
ATOM    810  N   ARG   119      46.613  12.961  47.780  1.00 25.93      B
ATOM    811  CA  ARG   119      46.922  13.355  46.423  1.00 26.49      B
ATOM    812  CB  ARG   119      47.076  14.913  46.313  1.00 24.19      B
ATOM    813  CG  ARG   119      45.824  15.737  46.642  1.00 18.83      B
ATOM    814  CD  ARG   119      44.579  15.206  45.965  1.00 15.06      B
ATOM    815  NE  ARG   119      44.755  14.940  44.542  1.00 15.80      B
ATOM    816  CZ  ARG   119      44.761  15.869  43.591  1.00 18.90      B
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ATOM	817	NH1	ARG	119	44.601	17.142	43.910	1.00	20.61	B
ATOM	818	NH2	ARG	119	44.910	15.528	42.314	1.00	17.87	B
ATOM	819	C	ARG	119	48.207	12.682	45.967	1.00	29.08	B
ATOM	820	O	ARG	119	49.178	12.572	46.735	1.00	27.84	B
ATOM	821	N	SER	120	48.205	12.192	44.731	1.00	30.37	B
ATOM	822	CA	SER	120	49.417	11.597	44.203	1.00	32.15	B
ATOM	823	CB	SER	120	49.190	11.014	42.825	1.00	33.55	B
ATOM	824	OG	SER	120	48.380	9.854	42.897	1.00	34.65	B
ATOM	825	C	SER	120	50.287	12.839	44.123	1.00	31.39	B
ATOM	826	O	SER	120	49.849	13.883	43.651	1.00	31.19	B
ATOM	827	N	PRO	121	51.522	12.745	44.599	1.00	30.67	B
ATOM	828	CD	PRO	121	52.207	11.494	44.965	1.00	31.67	B
ATOM	829	CA	PRO	121	52.455	13.870	44.595	1.00	31.71	B
ATOM	830	CB	PRO	121	53.674	13.288	45.270	1.00	31.87	B
ATOM	831	CG	PRO	121	53.658	11.869	44.783	1.00	32.88	B
ATOM	832	C	PRO	121	52.788	14.511	43.240	1.00	32.30	B
ATOM	833	O	PRO	121	52.557	13.925	42.176	1.00	32.32	B
ATOM	834	N	ASN	122	53.319	15.733	43.319	1.00	30.43	B
ATOM	835	CA	ASN	122	53.753	16.529	42.175	1.00	30.58	B
ATOM	836	CB	ASN	122	54.974	15.864	41.515	1.00	30.83	B
ATOM	837	CG	ASN	122	56.101	16.850	41.250	1.00	29.55	B
ATOM	838	OD1	ASN	122	56.512	17.589	42.139	1.00	30.20	B
ATOM	839	ND2	ASN	122	56.614	16.849	40.032	1.00	29.25	B
ATOM	840	C	ASN	122	52.708	16.838	41.107	1.00	30.96	B
ATOM	841	O	ASN	122	53.022	16.840	39.916	1.00	28.89	B
ATOM	842	N	GLU	123	51.479	17.121	41.540	1.00	31.29	B
ATOM	843	CA	GLU	123	50.380	17.435	40.630	1.00	31.61	B
ATOM	844	CB	GLU	123	50.437	18.873	40.222	1.00	29.75	B
ATOM	845	CG	GLU	123	50.311	19.825	41.382	1.00	31.53	B
ATOM	846	CD	GLU	123	50.030	21.243	40.942	1.00	34.00	B
ATOM	847	OE1	GLU	123	50.896	21.842	40.255	1.00	32.81	B
ATOM	848	OE2	GLU	123	48.937	21.753	41.288	1.00	35.74	B
ATOM	849	C	GLU	123	50.396	16.558	39.393	1.00	32.07	B
ATOM	850	O	GLU	123	50.246	17.038	38.272	1.00	32.39	B
ATOM	851	N	GLU	124	50.576	15.261	39.620	1.00	33.92	B
ATOM	852	CA	GLU	124	50.628	14.269	38.558	1.00	33.69	B
ATOM	853	CB	GLU	124	51.235	12.998	39.111	1.00	35.39	B
ATOM	854	CG	GLU	124	51.234	11.798	38.184	1.00	39.45	B
ATOM	855	CD	GLU	124	51.966	10.613	38.801	1.00	42.18	B
ATOM	856	OE1	GLU	124	51.802	10.390	40.026	1.00	42.52	B
ATOM	857	OE2	GLU	124	52.698	9.906	38.067	1.00	42.46	B
ATOM	858	C	GLU	124	49.252	13.994	37.958	1.00	33.48	B
ATOM	859	O	GLU	124	49.149	13.665	36.778	1.00	33.85	B
ATOM	860	N	TYR	125	48.196	14.141	38.758	1.00	32.64	B
ATOM	861	CA	TYR	125	46.841	13.895	38.267	1.00	33.52	B
ATOM	862	CB	TYR	125	46.261	12.523	38.817	1.00	33.48	B
ATOM	863	CG	TYR	125	47.109	11.290	38.613	1.00	35.23	B
ATOM	864	CD1	TYR	125	47.951	10.826	39.624	1.00	35.75	B
ATOM	865	CE1	TYR	125	48.709	9.668	39.461	1.00	36.41	B
ATOM	866	CD2	TYR	125	47.046	10.565	37.422	1.00	36.88	B
ATOM	867	CE2	TYR	125	47.803	9.403	37.242	1.00	37.22	B
ATOM	868	CZ	TYR	125	48.630	8.962	38.268	1.00	38.72	B
ATOM	869	OH	TYR	125	49.369	7.811	38.108	1.00	40.27	B
ATOM	870	C	TYR	125	45.851	14.985	38.677	1.00	33.79	B
ATOM	871	O	TYR	125	46.150	15.834	39.520	1.00	34.63	B
ATOM	872	N	THR	126	44.669	14.949	38.063	1.00	33.04	B
ATOM	873	CA	THR	126	43.588	15.858	38.420	1.00	31.85	B
ATOM	874	CB	THR	126	42.562	16.061	37.286	1.00	31.42	B
ATOM	875	OG1	THR	126	42.214	14.790	36.723	1.00	29.37	B
ATOM	876	CG2	THR	126	43.114	16.996	36.216	1.00	30.94	B
ATOM	877	C	THR	126	42.911	15.061	39.518	1.00	31.76	B
ATOM	878	O	THR	126	43.023	13.836	39.552	1.00	31.47	B
ATOM	879	N	TRP	127	42.197	15.738	40.401	1.00	31.44	B
ATOM	880	CA	TRP	127	41.559	15.053	41.507	1.00	30.17	B
ATOM	881	CB	TRP	127	40.749	16.048	42.357	1.00	27.67	B
ATOM	882	CG	TRP	127	39.474	16.455	41.718	1.00	25.01	B
ATOM	883	CD2	TRP	127	38.207	15.796	41.846	1.00	24.45	B
ATOM	884	CE2	TRP	127	37.285	16.514	41.059	1.00	24.12	B
ATOM	885	CE3	TRP	127	37.764	14.662	42.546	1.00	22.04	B
ATOM	886	CD1	TRP	127	39.278	17.507	40.885	1.00	23.64	B
ATOM	887	NE1	TRP	127	37.966	17.553	40.483	1.00	24.14	B
ATOM	888	CZ2	TRP	127	35.937	16.143	40.952	1.00	25.81	B
ATOM	889	CZ3	TRP	127	36.427	14.285	42.441	1.00	24.07	B

ATOM	890	CH2	TRP	127	35.526	15.026	41.647	1.00	26.19	B
ATOM	891	C	TRP	127	40.664	13.883	41.099	1.00	30.31	B
ATOM	892	O	TRP	127	40.635	12.859	41.784	1.00	31.25	B
ATOM	893	N	GLU	128	39.945	14.014	39.991	1.00	30.25	B
ATOM	894	CA	GLU	128	39.036	12.943	39.575	1.00	29.93	B
ATOM	895	CB	GLU	128	38.010	13.477	38.601	1.00	30.66	B
ATOM	896	CG	GLU	128	38.597	14.116	37.360	1.00	32.82	B
ATOM	897	CD	GLU	128	37.522	14.757	36.522	1.00	37.02	B
ATOM	898	OE1	GLU	128	36.740	15.558	37.085	1.00	37.94	B
ATOM	899	OE2	GLU	128	37.450	14.460	35.309	1.00	39.71	B
ATOM	900	C	GLU	128	39.692	11.704	38.977	1.00	28.41	B
ATOM	901	O	GLU	128	39.004	10.755	38.623	1.00	28.40	B
ATOM	902	N	GLU	129	41.012	11.716	38.853	1.00	27.73	B
ATOM	903	CA	GLU	129	41.724	10.574	38.303	1.00	26.98	B
ATOM	904	CB	GLU	129	42.343	10.919	36.940	1.00	25.80	B
ATOM	905	CG	GLU	129	41.317	11.144	35.841	1.00	28.03	B
ATOM	906	CD	GLU	129	41.954	11.422	34.487	1.00	33.17	B
ATOM	907	OE1	GLU	129	41.201	11.654	33.510	1.00	35.80	B
ATOM	908	OE2	GLU	129	43.206	11.411	34.389	1.00	33.91	B
ATOM	909	C	GLU	129	42.807	10.110	39.257	1.00	27.19	B
ATOM	910	O	GLU	129	43.480	9.117	38.997	1.00	28.14	B
ATOM	911	N	ASP	130	42.966	10.814	40.372	1.00	27.13	B
ATOM	912	CA	ASP	130	43.995	10.445	41.336	1.00	28.16	B
ATOM	913	CB	ASP	130	44.092	11.498	42.458	1.00	29.19	B
ATOM	914	CG	ASP	130	45.484	11.577	43.061	1.00	31.28	B
ATOM	915	OD1	ASP	130	46.026	10.525	43.470	1.00	31.52	B
ATOM	916	OD2	ASP	130	46.039	12.695	43.125	1.00	33.01	B
ATOM	917	C	ASP	130	43.690	9.068	41.925	1.00	27.22	B
ATOM	918	O	ASP	130	42.646	8.865	42.551	1.00	27.12	B
ATOM	919	N	PRO	131	44.590	8.093	41.704	1.00	26.27	B
ATOM	920	CD	PRO	131	45.722	8.143	40.760	1.00	25.74	B
ATOM	921	CA	PRO	131	44.404	6.733	42.217	1.00	25.42	B
ATOM	922	CB	PRO	131	45.436	5.928	41.431	1.00	25.20	B
ATOM	923	CG	PRO	131	46.516	6.926	41.158	1.00	25.28	B
ATOM	924	C	PRO	131	44.550	6.586	43.734	1.00	25.10	B
ATOM	925	O	PRO	131	44.317	5.514	44.284	1.00	25.70	B
ATOM	926	N	LEU	132	44.939	7.659	44.414	1.00	25.55	B
ATOM	927	CA	LEU	132	45.061	7.615	45.870	1.00	24.12	B
ATOM	928	CB	LEU	132	46.335	8.393	46.358	1.00	23.33	B
ATOM	929	CG	LEU	132	47.750	7.835	45.985	1.00	24.01	B
ATOM	930	CD1	LEU	132	48.853	8.699	46.613	1.00	21.35	B
ATOM	931	CD2	LEU	132	47.875	6.394	46.474	1.00	25.49	B
ATOM	932	C	LEU	132	43.794	8.216	46.497	1.00	23.99	B
ATOM	933	O	LEU	132	43.694	8.338	47.728	1.00	24.50	B
ATOM	934	N	ALA	133	42.831	8.587	45.650	1.00	21.97	B
ATOM	935	CA	ALA	133	41.566	9.155	46.129	1.00	23.50	B
ATOM	936	CB	ALA	133	40.738	9.710	44.958	1.00	19.96	B
ATOM	937	C	ALA	133	40.760	8.097	46.896	1.00	24.12	B
ATOM	938	O	ALA	133	40.766	6.914	46.552	1.00	24.63	B
ATOM	939	N	GLY	134	40.060	8.546	47.931	1.00	25.21	B
ATOM	940	CA	GLY	134	39.289	7.646	48.763	1.00	23.61	B
ATOM	941	C	GLY	134	37.831	7.541	48.387	1.00	23.90	B
ATOM	942	O	GLY	134	37.399	8.030	47.344	1.00	25.12	B
ATOM	943	N	ILE	135	37.075	6.887	49.261	1.00	22.33	B
ATOM	944	CA	ILE	135	35.657	6.662	49.055	1.00	19.60	B
ATOM	945	CB	ILE	135	35.048	5.962	50.295	1.00	17.94	B
ATOM	946	CG2	ILE	135	33.513	5.984	50.232	1.00	15.17	B
ATOM	947	CG1	ILE	135	35.604	4.531	50.381	1.00	13.85	B
ATOM	948	CD1	ILE	135	35.402	3.883	51.712	1.00	11.57	B
ATOM	949	C	ILE	135	34.886	7.941	48.751	1.00	19.64	B
ATOM	950	O	ILE	135	34.130	7.995	47.789	1.00	17.27	B
ATOM	951	N	ILE	136	35.090	8.971	49.566	1.00	19.64	B
ATOM	952	CA	ILE	136	34.383	10.229	49.377	1.00	19.00	B
ATOM	953	CB	ILE	136	34.758	11.219	50.486	1.00	18.34	B
ATOM	954	CG2	ILE	136	34.174	12.595	50.188	1.00	19.49	B
ATOM	955	CG1	ILE	136	34.226	10.669	51.838	1.00	18.91	B
ATOM	956	CD1	ILE	136	34.680	11.447	53.086	1.00	18.92	B
ATOM	957	C	ILE	136	34.552	10.867	47.991	1.00	17.37	B
ATOM	958	O	ILE	136	33.614	10.888	47.207	1.00	15.94	B
ATOM	959	N	PRO	137	35.742	11.382	47.662	1.00	16.74	B
ATOM	960	CD	PRO	137	37.083	11.311	48.259	1.00	16.29	B
ATOM	961	CA	PRO	137	35.785	11.963	46.318	1.00	17.68	B
ATOM	962	CB	PRO	137	37.263	12.305	46.132	1.00	14.17	B

ATOM	963	CG	PRO	137	37.966	11.351	47.037	1.00	16.06	B
ATOM	964	C	PRO	137	35.229	11.025	45.232	1.00	20.66	B
ATOM	965	O	PRO	137	34.408	11.434	44.406	1.00	22.43	B
ATOM	966	N	ARG	138	35.651	9.764	45.232	1.00	21.33	B
ATOM	967	CA	ARG	138	35.154	8.825	44.224	1.00	21.16	B
ATOM	968	CB	ARG	138	35.768	7.428	44.436	1.00	19.87	B
ATOM	969	CG	ARG	138	37.251	7.370	44.138	1.00	18.07	B
ATOM	970	CD	ARG	138	37.812	5.989	44.402	1.00	17.00	B
ATOM	971	NE	ARG	138	39.264	6.019	44.408	1.00	14.48	B
ATOM	972	CZ	ARG	138	40.016	5.909	43.327	1.00	16.26	B
ATOM	973	NH1	ARG	138	39.446	5.743	42.137	1.00	15.29	B
ATOM	974	NH2	ARG	138	41.337	6.004	43.433	1.00	14.85	B
ATOM	975	C	ARG	138	33.630	8.705	44.202	1.00	21.32	B
ATOM	976	O	ARG	138	33.021	8.644	43.139	1.00	25.00	B
ATOM	977	N	THR	139	33.009	8.667	45.370	1.00	20.40	B
ATOM	978	CA	THR	139	31.562	8.540	45.436	1.00	20.86	B
ATOM	979	CB	THR	139	31.081	8.385	46.895	1.00	20.11	B
ATOM	980	OG1	THR	139	31.770	7.293	47.512	1.00	21.18	B
ATOM	981	CG2	THR	139	29.583	8.120	46.944	1.00	18.68	B
ATOM	982	C	THR	139	30.883	9.753	44.815	1.00	23.10	B
ATOM	983	O	THR	139	29.955	9.613	44.014	1.00	24.95	B
ATOM	984	N	LEU	140	31.340	10.944	45.189	1.00	23.71	B
ATOM	985	CA	LEU	140	30.762	12.175	44.659	1.00	23.38	B
ATOM	986	CB	LEU	140	31.480	13.401	45.238	1.00	21.47	B
ATOM	987	CG	LEU	140	31.211	13.560	46.733	1.00	21.91	B
ATOM	988	CD1	LEU	140	32.120	14.621	47.305	1.00	21.37	B
ATOM	989	CD2	LEU	140	29.740	13.883	46.966	1.00	18.69	B
ATOM	990	C	LEU	140	30.859	12.184	43.154	1.00	23.10	B
ATOM	991	O	LEU	140	29.870	12.395	42.467	1.00	21.86	B
ATOM	992	N	HIS	141	32.058	11.948	42.645	1.00	24.02	B
ATOM	993	CA	HIS	141	32.272	11.927	41.207	1.00	27.46	B
ATOM	994	CB	HIS	141	33.741	11.616	40.908	1.00	27.50	B
ATOM	995	CG	HIS	141	34.101	11.718	39.457	1.00	30.18	B
ATOM	996	CD2	HIS	141	34.041	10.807	38.457	1.00	30.98	B
ATOM	997	ND1	HIS	141	34.614	12.869	38.896	1.00	30.79	B
ATOM	998	CE1	HIS	141	34.859	12.662	37.615	1.00	29.68	B
ATOM	999	NE2	HIS	141	34.520	11.419	37.324	1.00	31.87	B
ATOM	1000	C	HIS	141	31.372	10.885	40.517	1.00	28.79	B
ATOM	1001	O	HIS	141	30.835	11.133	39.432	1.00	30.63	B
ATOM	1002	N	GLN	142	31.196	9.728	41.154	1.00	27.09	B
ATOM	1003	CA	GLN	142	30.392	8.664	40.579	1.00	26.11	B
ATOM	1004	CB	GLN	142	30.660	7.381	41.302	1.00	27.58	B
ATOM	1005	CG	GLN	142	31.938	6.733	40.855	1.00	29.72	B
ATOM	1006	CD	GLN	142	32.001	6.617	39.344	1.00	31.15	B
ATOM	1007	OE1	GLN	142	31.181	5.929	38.729	1.00	32.85	B
ATOM	1008	NE2	GLN	142	32.969	7.300	38.735	1.00	29.44	B
ATOM	1009	C	GLN	142	28.894	8.913	40.514	1.00	25.79	B
ATOM	1010	O	GLN	142	28.238	8.494	39.564	1.00	25.19	B
ATOM	1011	N	ILE	143	28.351	9.583	41.523	1.00	24.49	B
ATOM	1012	CA	ILE	143	26.928	9.888	41.555	1.00	23.07	B
ATOM	1013	CB	ILE	143	26.581	10.716	42.805	1.00	22.41	B
ATOM	1014	CG2	ILE	143	25.174	11.285	42.690	1.00	24.89	B
ATOM	1015	CG1	ILE	143	26.727	9.856	44.044	1.00	21.77	B
ATOM	1016	CD1	ILE	143	26.477	10.599	45.339	1.00	21.34	B
ATOM	1017	C	ILE	143	26.492	10.664	40.308	1.00	23.84	B
ATOM	1018	O	ILE	143	25.417	10.425	39.769	1.00	23.49	B
ATOM	1019	N	PHE	144	27.334	11.593	39.860	1.00	25.75	B
ATOM	1020	CA	PHE	144	27.044	12.418	38.690	1.00	27.59	B
ATOM	1021	CB	PHE	144	28.019	13.657	38.638	1.00	26.93	B
ATOM	1022	CG	PHE	144	27.734	14.694	39.688	1.00	27.63	B
ATOM	1023	CD1	PHE	144	26.583	15.478	39.614	1.00	28.58	B
ATOM	1024	CD2	PHE	144	28.577	14.845	40.785	1.00	27.80	B
ATOM	1025	CE1	PHE	144	26.271	16.396	40.626	1.00	28.69	B
ATOM	1026	CE2	PHE	144	28.279	15.756	41.802	1.00	27.42	B
ATOM	1027	CZ	PHE	144	27.121	16.532	41.723	1.00	29.86	B
ATOM	1028	C	PHE	144	27.129	11.621	37.394	1.00	28.56	B
ATOM	1029	O	PHE	144	26.425	11.918	36.423	1.00	27.83	B
ATOM	1030	N	GLU	145	27.998	10.614	37.382	1.00	30.60	B
ATOM	1031	CA	GLU	145	28.160	9.757	36.209	1.00	32.75	B
ATOM	1032	CB	GLU	145	29.433	8.889	36.357	1.00	35.85	B
ATOM	1033	CG	GLU	145	30.742	9.673	36.317	1.00	42.03	B
ATOM	1034	CD	GLU	145	31.201	9.977	34.898	1.00	46.55	B
ATOM	1035	OE1	GLU	145	32.014	10.916	34.699	1.00	47.36	B

ATOM	1036	OE2	GLU	145	30.748	9.262	33.976	1.00	49.72	B
ATOM	1037	C	GLU	145	26.934	8.854	36.040	1.00	32.32	B
ATOM	1038	O	GLU	145	26.319	8.812	34.974	1.00	32.21	B
ATOM	1039	N	LYS	146	26.573	8.150	37.104	1.00	31.79	B
ATOM	1040	CA	LYS	146	25.443	7.235	37.066	1.00	34.10	B
ATOM	1041	CB	LYS	146	25.340	6.463	38.430	1.00	34.57	B
ATOM	1042	CG	LYS	146	26.693	5.973	38.952	1.00	35.68	B
ATOM	1043	CD	LYS	146	26.597	4.862	39.994	1.00	34.50	B
ATOM	1044	CE	LYS	146	26.566	3.486	39.327	1.00	35.54	B
ATOM	1045	NZ	LYS	146	27.115	2.405	40.204	1.00	33.09	B
ATOM	1046	C	LYS	146	24.098	7.888	36.721	1.00	34.95	B
ATOM	1047	O	LYS	146	23.320	7.342	35.929	1.00	35.60	B
ATOM	1048	N	LEU	147	23.831	9.057	37.298	1.00	34.40	B
ATOM	1049	CA	LEU	147	22.574	9.762	37.061	1.00	33.66	B
ATOM	1050	CB	LEU	147	22.154	10.477	38.336	1.00	32.95	B
ATOM	1051	CG	LEU	147	21.963	9.607	39.554	1.00	33.64	B
ATOM	1052	CD1	LEU	147	21.682	10.474	40.775	1.00	34.40	B
ATOM	1053	CD2	LEU	147	20.809	8.645	39.308	1.00	35.51	B
ATOM	1054	C	LEU	147	22.634	10.772	35.907	1.00	34.15	B
ATOM	1055	O	LEU	147	21.724	11.576	35.728	1.00	32.96	B
ATOM	1056	N	THR	148	23.698	10.719	35.115	1.00	35.64	B
ATOM	1057	CA	THR	148	23.863	11.656	34.011	1.00	36.46	B
ATOM	1058	CB	THR	148	25.138	11.332	33.198	1.00	35.78	B
ATOM	1059	OG1	THR	148	25.492	12.468	32.409	1.00	36.67	B
ATOM	1060	CG2	THR	148	24.914	10.150	32.274	1.00	36.63	B
ATOM	1061	C	THR	148	22.659	11.770	33.057	1.00	37.44	B
ATOM	1062	O	THR	148	22.313	12.878	32.639	1.00	37.93	B
ATOM	1063	N	ASP	149	22.019	10.653	32.712	1.00	35.78	B
ATOM	1064	CA	ASP	149	20.867	10.706	31.807	1.00	35.94	B
ATOM	1065	CB	ASP	149	21.337	11.004	30.322	1.00	34.77	B
ATOM	1066	CG	ASP	149	22.404	10.027	29.827	1.00	36.65	B
ATOM	1067	OD1	ASP	149	22.605	8.965	30.467	1.00	35.17	B
ATOM	1068	OD2	ASP	149	23.032	10.321	28.784	1.00	35.41	B
ATOM	1069	C	ASP	149	19.966	9.460	31.824	1.00	36.15	B
ATOM	1070	O	ASP	149	19.568	8.947	30.769	1.00	32.78	B
ATOM	1071	N	ASN	150	19.639	8.987	33.025	1.00	36.51	B
ATOM	1072	CA	ASN	150	18.781	7.819	33.181	1.00	38.16	B
ATOM	1073	CB	ASN	150	19.218	6.992	34.417	1.00	37.97	B
ATOM	1074	CG	ASN	150	19.159	7.785	35.704	1.00	37.13	B
ATOM	1075	OD1	ASN	150	19.548	8.951	35.742	1.00	37.20	B
ATOM	1076	ND2	ASN	150	18.694	7.148	36.774	1.00	36.82	B
ATOM	1077	C	ASN	150	17.314	8.240	33.305	1.00	39.47	B
ATOM	1078	O	ASN	150	16.419	7.397	33.433	1.00	39.49	B
ATOM	1079	N	GLY	151	17.077	9.549	33.245	1.00	39.29	B
ATOM	1080	CA	GLY	151	15.725	10.063	33.343	1.00	39.01	B
ATOM	1081	C	GLY	151	15.333	10.349	34.772	1.00	39.23	B
ATOM	1082	O	GLY	151	14.170	10.612	35.063	1.00	40.53	B
ATOM	1083	N	THR	152	16.307	10.285	35.670	1.00	40.25	B
ATOM	1084	CA	THR	152	16.069	10.547	37.085	1.00	40.87	B
ATOM	1085	CB	THR	152	16.730	9.463	37.960	1.00	39.78	B
ATOM	1086	OG1	THR	152	16.146	8.191	37.655	1.00	43.27	B
ATOM	1087	CG2	THR	152	16.531	9.764	39.437	1.00	40.09	B
ATOM	1088	C	THR	152	16.643	11.918	37.448	1.00	41.24	B
ATOM	1089	O	THR	152	17.860	12.120	37.434	1.00	42.84	B
ATOM	1090	N	GLU	153	15.753	12.856	37.754	1.00	40.50	B
ATOM	1091	CA	GLU	153	16.140	14.216	38.118	1.00	39.45	B
ATOM	1092	CB	GLU	153	14.910	15.143	38.054	1.00	41.77	B
ATOM	1093	CG	GLU	153	15.258	16.606	37.831	1.00	47.08	B
ATOM	1094	CD	GLU	153	15.903	16.847	36.474	1.00	49.24	B
ATOM	1095	OE1	GLU	153	16.559	17.901	36.313	1.00	49.10	B
ATOM	1096	OE2	GLU	153	15.747	15.988	35.570	1.00	49.10	B
ATOM	1097	C	GLU	153	16.697	14.170	39.538	1.00	36.82	B
ATOM	1098	O	GLU	153	16.140	13.472	40.387	1.00	35.59	B
ATOM	1099	N	PHE	154	17.770	14.919	39.807	1.00	33.77	B
ATOM	1100	CA	PHE	154	18.380	14.877	41.140	1.00	31.58	B
ATOM	1101	CB	PHE	154	19.302	13.644	41.212	1.00	29.10	B
ATOM	1102	CG	PHE	154	20.572	13.797	40.414	1.00	25.93	B
ATOM	1103	CD1	PHE	154	21.763	14.165	41.038	1.00	25.72	B
ATOM	1104	CD2	PHE	154	20.573	13.597	39.037	1.00	23.66	B
ATOM	1105	CE1	PHE	154	22.941	14.328	40.297	1.00	26.03	B
ATOM	1106	CE2	PHE	154	21.741	13.758	38.294	1.00	25.52	B
ATOM	1107	CZ	PHE	154	22.930	14.123	38.925	1.00	24.44	B
ATOM	1108	C	PHE	154	19.183	16.093	41.627	1.00	29.93	B

ATOM	1109	O	PHE	154	19.651	16.924	40.850	1.00	30.00	B
ATOM	1110	N	SER	155	19.357	16.157	42.940	1.00	28.97	B
ATOM	1111	CA	SER	155	20.140	17.212	43.572	1.00	28.90	B
ATOM	1112	CB	SER	155	19.225	18.281	44.243	1.00	26.53	B
ATOM	1113	OG	SER	155	18.732	17.844	45.502	1.00	24.48	B
ATOM	1114	C	SER	155	21.010	16.537	44.635	1.00	28.97	B
ATOM	1115	O	SER	155	20.588	15.569	45.279	1.00	28.86	B
ATOM	1116	N	VAL	156	22.221	17.047	44.819	1.00	29.35	B
ATOM	1117	CA	VAL	156	23.135	16.483	45.803	1.00	29.64	B
ATOM	1118	CB	VAL	156	24.431	15.977	45.125	1.00	28.79	B
ATOM	1119	CG1	VAL	156	25.280	15.208	46.124	1.00	29.92	B
ATOM	1120	CG2	VAL	156	24.089	15.116	43.930	1.00	29.12	B
ATOM	1121	C	VAL	156	23.516	17.517	46.863	1.00	29.76	B
ATOM	1122	O	VAL	156	23.925	18.627	46.532	1.00	30.11	B
ATOM	1123	N	LYS	157	23.372	17.149	48.132	1.00	30.23	B
ATOM	1124	CA	LYS	157	23.731	18.028	49.245	1.00	31.02	B
ATOM	1125	CB	LYS	157	22.489	18.431	50.063	1.00	32.19	B
ATOM	1126	CG	LYS	157	21.543	19.376	49.364	1.00	35.38	B
ATOM	1127	CD	LYS	157	20.246	19.523	50.162	1.00	39.38	B
ATOM	1128	CE	LYS	157	19.169	20.259	49.369	1.00	39.91	B
ATOM	1129	NZ	LYS	157	17.857	20.187	50.067	1.00	40.45	B
ATOM	1130	C	LYS	157	24.702	17.308	50.171	1.00	30.04	B
ATOM	1131	O	LYS	157	24.399	16.230	50.668	1.00	30.82	B
ATOM	1132	N	VAL	158	25.866	17.900	50.402	1.00	27.97	B
ATOM	1133	CA	VAL	158	26.839	17.290	51.292	1.00	27.63	B
ATOM	1134	CB	VAL	158	28.284	17.406	50.751	1.00	27.29	B
ATOM	1135	CG1	VAL	158	28.433	16.582	49.478	1.00	29.26	B
ATOM	1136	CG2	VAL	158	28.632	18.861	50.491	1.00	26.29	B
ATOM	1137	C	VAL	158	26.785	17.959	52.649	1.00	27.62	B
ATOM	1138	O	VAL	158	26.182	19.009	52.818	1.00	27.51	B
ATOM	1139	N	SER	159	27.431	17.344	53.624	1.00	28.77	B
ATOM	1140	CA	SER	159	27.449	17.896	54.962	1.00	29.25	B
ATOM	1141	CB	SER	159	26.155	17.634	55.612	1.00	29.36	B
ATOM	1142	OG	SER	159	26.083	18.324	56.835	1.00	35.64	B
ATOM	1143	C	SER	159	28.584	17.255	55.753	1.00	28.48	B
ATOM	1144	O	SER	159	28.762	16.037	55.723	1.00	29.46	B
ATOM	1145	N	LEU	160	29.364	18.070	56.451	1.00	26.66	B
ATOM	1146	CA	LEU	160	30.473	17.529	57.215	1.00	26.24	B
ATOM	1147	CB	LEU	160	31.769	18.008	56.649	1.00	26.22	B
ATOM	1148	CG	LEU	160	33.024	17.381	57.255	1.00	25.56	B
ATOM	1149	CD1	LEU	160	32.850	15.873	57.350	1.00	24.56	B
ATOM	1150	CD2	LEU	160	34.241	17.759	56.400	1.00	24.75	B
ATOM	1151	C	LEU	160	30.393	17.872	58.690	1.00	26.51	B
ATOM	1152	O	LEU	160	30.816	18.949	59.119	1.00	24.86	B
ATOM	1153	N	LEU	161	29.844	16.937	59.461	1.00	25.32	B
ATOM	1154	CA	LEU	161	29.686	17.112	60.895	1.00	23.81	B
ATOM	1155	CB	LEU	161	28.349	16.607	61.310	1.00	23.24	B
ATOM	1156	CG	LEU	161	28.109	16.490	62.766	1.00	23.19	B
ATOM	1157	CD1	LEU	161	27.992	17.879	63.371	1.00	24.82	B
ATOM	1158	CD2	LEU	161	26.838	15.701	62.989	1.00	22.84	B
ATOM	1159	C	LEU	161	30.777	16.338	61.613	1.00	24.19	B
ATOM	1160	O	LEU	161	31.024	15.178	61.307	1.00	25.43	B
ATOM	1161	N	GLU	162	31.444	16.983	62.563	1.00	23.56	B
ATOM	1162	CA	GLU	162	32.507	16.322	63.304	1.00	21.29	B
ATOM	1163	CB	GLU	162	33.892	16.895	62.872	1.00	19.65	B
ATOM	1164	CG	GLU	162	34.027	16.956	61.338	1.00	18.31	B
ATOM	1165	CD	GLU	162	35.463	16.923	60.845	1.00	19.90	B
ATOM	1166	OE1	GLU	162	36.362	17.416	61.557	1.00	20.88	B
ATOM	1167	OE2	GLU	162	35.699	16.413	59.729	1.00	21.08	B
ATOM	1168	C	GLU	162	32.276	16.448	64.803	1.00	21.51	B
ATOM	1169	O	GLU	162	31.734	17.441	65.286	1.00	24.11	B
ATOM	1170	N	ILE	163	32.665	15.419	65.543	1.00	20.50	B
ATOM	1171	CA	ILE	163	32.464	15.414	66.979	1.00	16.52	B
ATOM	1172	CB	ILE	163	31.587	14.221	67.396	1.00	15.68	B
ATOM	1173	CG2	ILE	163	31.070	14.412	68.813	1.00	13.11	B
ATOM	1174	CG1	ILE	163	30.420	14.093	66.427	1.00	14.88	B
ATOM	1175	CD1	ILE	163	29.521	12.920	66.704	1.00	16.15	B
ATOM	1176	C	ILE	163	33.805	15.325	67.672	1.00	17.43	B
ATOM	1177	O	ILE	163	34.644	14.499	67.319	1.00	17.59	B
ATOM	1178	N	TYR	164	33.996	16.201	68.654	1.00	17.46	B
ATOM	1179	CA	TYR	164	35.219	16.263	69.430	1.00	16.57	B
ATOM	1180	CB	TYR	164	36.192	17.276	68.783	1.00	14.70	B
ATOM	1181	CG	TYR	164	37.464	17.474	69.559	1.00	12.25	B

ATOM	1182	CD1	TYR	164	37.502	18.334	70.653	1.00	13.17	B
ATOM	1183	CE1	TYR	164	38.643	18.439	71.454	1.00	15.94	B
ATOM	1184	CD2	TYR	164	38.600	16.724	69.267	1.00	13.00	B
ATOM	1185	CE2	TYR	164	39.753	16.814	70.058	1.00	15.22	B
ATOM	1186	CZ	TYR	164	39.773	17.674	71.155	1.00	17.31	B
ATOM	1187	OH	TYR	164	40.909	17.774	71.952	1.00	15.71	B
ATOM	1188	C	TYR	164	34.875	16.669	70.863	1.00	18.56	B
ATOM	1189	O	TYR	164	34.289	17.726	71.094	1.00	21.94	B
ATOM	1190	N	ASN	165	35.225	15.826	71.828	1.00	20.33	B
ATOM	1191	CA	ASN	165	34.942	16.122	73.232	1.00	22.94	B
ATOM	1192	CB	ASN	165	35.633	17.402	73.653	1.00	24.28	B
ATOM	1193	CG	ASN	165	36.418	17.255	74.942	1.00	28.53	B
ATOM	1194	OD1	ASN	165	37.598	16.864	74.929	1.00	31.28	B
ATOM	1195	ND2	ASN	165	35.777	17.569	76.064	1.00	24.86	B
ATOM	1196	C	ASN	165	33.443	16.314	73.406	1.00	24.90	B
ATOM	1197	O	ASN	165	33.009	17.222	74.121	1.00	26.77	B
ATOM	1198	N	GLU	166	32.657	15.471	72.745	1.00	23.40	B
ATOM	1199	CA	GLU	166	31.200	15.555	72.813	1.00	22.69	B
ATOM	1200	CB	GLU	166	30.706	15.231	74.237	1.00	22.07	B
ATOM	1201	CG	GLU	166	30.814	13.757	74.590	1.00	22.71	B
ATOM	1202	CD	GLU	166	30.157	12.849	73.548	1.00	23.19	B
ATOM	1203	OE1	GLU	166	28.906	12.779	73.505	1.00	22.44	B
ATOM	1204	OE2	GLU	166	30.899	12.211	72.769	1.00	21.71	B
ATOM	1205	C	GLU	166	30.610	16.884	72.349	1.00	22.21	B
ATOM	1206	O	GLU	166	29.491	17.228	72.709	1.00	22.53	B
ATOM	1207	N	GLU	167	31.363	17.631	71.545	1.00	24.18	B
ATOM	1208	CA	GLU	167	30.885	18.899	71.011	1.00	23.58	B
ATOM	1209	CB	GLU	167	31.825	20.009	71.365	1.00	28.43	B
ATOM	1210	CG	GLU	167	31.900	20.321	72.848	1.00	34.21	B
ATOM	1211	CD	GLU	167	32.857	21.470	73.142	1.00	40.07	B
ATOM	1212	OE1	GLU	167	34.033	21.400	72.702	1.00	41.07	B
ATOM	1213	OE2	GLU	167	32.431	22.441	73.812	1.00	43.47	B
ATOM	1214	C	GLU	167	30.800	18.766	69.500	1.00	22.74	B
ATOM	1215	O	GLU	167	31.659	18.142	68.884	1.00	23.08	B
ATOM	1216	N	LEU	168	29.766	19.347	68.904	1.00	21.20	B
ATOM	1217	CA	LEU	168	29.578	19.274	67.461	1.00	20.52	B
ATOM	1218	CB	LEU	168	28.088	19.156	67.125	1.00	21.09	B
ATOM	1219	CG	LEU	168	27.319	17.889	67.681	1.00	22.11	B
ATOM	1220	CD1	LEU	168	28.249	16.663	67.622	1.00	15.69	B
ATOM	1221	CD2	LEU	168	26.837	18.136	69.114	1.00	21.13	B
ATOM	1222	C	LEU	168	30.173	20.458	66.702	1.00	21.77	B
ATOM	1223	O	LEU	168	30.178	21.598	67.179	1.00	22.45	B
ATOM	1224	N	PHE	169	30.673	20.171	65.506	1.00	20.28	B
ATOM	1225	CA	PHE	169	31.282	21.180	64.665	1.00	19.17	B
ATOM	1226	CB	PHE	169	32.835	21.112	64.778	1.00	19.31	B
ATOM	1227	CG	PHE	169	33.345	21.308	66.177	1.00	19.18	B
ATOM	1228	CD1	PHE	169	33.688	20.213	66.966	1.00	20.05	B
ATOM	1229	CD2	PHE	169	33.434	22.591	66.722	1.00	18.70	B
ATOM	1230	CE1	PHE	169	34.112	20.385	68.281	1.00	19.61	B
ATOM	1231	CE2	PHE	169	33.852	22.782	68.027	1.00	18.44	B
ATOM	1232	CZ	PHE	169	34.193	21.676	68.814	1.00	22.70	B
ATOM	1233	C	PHE	169	30.865	20.981	63.220	1.00	20.25	B
ATOM	1234	O	PHE	169	30.476	19.880	62.808	1.00	20.20	B
ATOM	1235	N	ASP	170	30.949	22.064	62.462	1.00	19.31	B
ATOM	1236	CA	ASP	170	30.603	22.069	61.053	1.00	19.06	B
ATOM	1237	CB	ASP	170	29.549	23.141	60.785	1.00	19.49	B
ATOM	1238	CG	ASP	170	28.970	23.066	59.386	1.00	21.37	B
ATOM	1239	OD1	ASP	170	29.648	22.556	58.463	1.00	20.46	B
ATOM	1240	OD2	ASP	170	27.827	23.542	59.206	1.00	24.10	B
ATOM	1241	C	ASP	170	31.902	22.429	60.353	1.00	20.21	B
ATOM	1242	O	ASP	170	32.402	23.540	60.509	1.00	21.52	B
ATOM	1243	N	LEU	171	32.460	21.492	59.599	1.00	20.15	B
ATOM	1244	CA	LEU	171	33.699	21.758	58.900	1.00	22.53	B
ATOM	1245	CB	LEU	171	34.620	20.517	58.965	1.00	19.76	B
ATOM	1246	CG	LEU	171	35.385	20.297	60.340	1.00	18.93	B
ATOM	1247	CD1	LEU	171	36.562	21.251	60.487	1.00	16.80	B
ATOM	1248	CD2	LEU	171	34.426	20.479	61.495	1.00	18.41	B
ATOM	1249	C	LEU	171	33.460	22.198	57.459	1.00	24.95	B
ATOM	1250	O	LEU	171	34.374	22.169	56.632	1.00	25.06	B
ATOM	1251	N	LEU	172	32.233	22.618	57.160	1.00	28.25	B
ATOM	1252	CA	LEU	172	31.910	23.081	55.812	1.00	33.55	B
ATOM	1253	CB	LEU	172	31.001	22.111	55.116	1.00	33.77	B
ATOM	1254	CG	LEU	172	31.664	20.867	54.556	1.00	34.20	B

ATOM	1255	CD1	LEU	172	30.632	20.056	53.783	1.00	33.48	B
ATOM	1256	CD2	LEU	172	32.807	21.268	53.644	1.00	34.44	B
ATOM	1257	C	LEU	172	31.279	24.461	55.766	1.00	35.97	B
ATOM	1258	O	LEU	172	31.181	25.059	54.706	1.00	37.85	B
ATOM	1259	N	ASN	173	30.843	24.962	56.912	1.00	39.07	B
ATOM	1260	CA	ASN	173	30.242	26.284	56.972	1.00	44.33	B
ATOM	1261	CB	ASN	173	29.451	26.445	58.275	1.00	45.10	B
ATOM	1262	CG	ASN	173	28.700	27.765	58.345	1.00	47.21	B
ATOM	1263	OD1	ASN	173	27.898	27.987	59.254	1.00	46.55	B
ATOM	1264	ND2	ASN	173	28.958	28.650	57.384	1.00	47.66	B
ATOM	1265	C	ASN	173	31.355	27.330	56.903	1.00	48.18	B
ATOM	1266	O	ASN	173	32.094	27.532	57.871	1.00	47.58	B
ATOM	1267	N	PRO	174	31.492	28.007	55.752	1.00	51.96	B
ATOM	1268	CD	PRO	174	30.737	27.802	54.502	1.00	52.92	B
ATOM	1269	CA	PRO	174	32.527	29.030	55.572	1.00	55.50	B
ATOM	1270	CB	PRO	174	32.609	29.162	54.076	1.00	54.73	B
ATOM	1271	CG	PRO	174	31.184	28.973	53.660	1.00	53.60	B
ATOM	1272	C	PRO	174	32.226	30.364	56.259	1.00	58.47	B
ATOM	1273	O	PRO	174	33.076	31.256	56.286	1.00	59.03	B
ATOM	1274	N	SER	175	31.024	30.497	56.819	1.00	60.76	B
ATOM	1275	CA	SER	175	30.639	31.730	57.504	1.00	62.73	B
ATOM	1276	CB	SER	175	29.138	32.013	57.301	1.00	63.76	B
ATOM	1277	OG	SER	175	28.877	32.450	55.975	1.00	66.00	B
ATOM	1278	C	SER	175	30.957	31.725	59.000	1.00	63.50	B
ATOM	1279	O	SER	175	30.901	32.769	59.654	1.00	63.94	B
ATOM	1280	N	SER	176	31.293	30.557	59.543	1.00	63.63	B
ATOM	1281	CA	SER	176	31.613	30.456	60.964	1.00	63.17	B
ATOM	1282	CB	SER	176	30.589	29.549	61.694	1.00	63.04	B
ATOM	1283	OG	SER	176	30.805	28.181	61.389	1.00	64.15	B
ATOM	1284	C	SER	176	33.017	29.909	61.188	1.00	62.90	B
ATOM	1285	O	SER	176	33.758	29.643	60.238	1.00	62.07	B
ATOM	1286	N	ASP	177	33.371	29.744	62.459	1.00	62.85	B
ATOM	1287	CA	ASP	177	34.676	29.225	62.837	1.00	62.62	B
ATOM	1288	CB	ASP	177	35.352	30.147	63.856	1.00	63.20	B
ATOM	1289	CG	ASP	177	35.504	31.559	63.345	1.00	63.21	B
ATOM	1290	OD1	ASP	177	36.062	31.729	62.243	1.00	63.09	B
ATOM	1291	OD2	ASP	177	35.068	32.498	64.044	1.00	62.91	B
ATOM	1292	C	ASP	177	34.515	27.852	63.452	1.00	61.87	B
ATOM	1293	O	ASP	177	33.447	27.504	63.954	1.00	62.79	B
ATOM	1294	N	VAL	178	35.588	27.078	63.415	1.00	60.45	B
ATOM	1295	CA	VAL	178	35.572	25.743	63.977	1.00	59.51	B
ATOM	1296	CB	VAL	178	36.894	25.005	63.688	1.00	59.52	B
ATOM	1297	CG1	VAL	178	37.118	24.909	62.183	1.00	59.92	B
ATOM	1298	CG2	VAL	178	38.048	25.729	64.356	1.00	59.97	B
ATOM	1299	C	VAL	178	35.363	25.834	65.485	1.00	58.12	B
ATOM	1300	O	VAL	178	35.159	24.825	66.157	1.00	59.80	B
ATOM	1301	N	SER	179	35.421	27.047	66.016	1.00	55.31	B
ATOM	1302	CA	SER	179	35.221	27.245	67.443	1.00	52.98	B
ATOM	1303	CB	SER	179	35.823	28.578	67.871	1.00	51.75	B
ATOM	1304	OG	SER	179	35.401	29.619	67.011	1.00	50.71	B
ATOM	1305	C	SER	179	33.725	27.211	67.746	1.00	52.04	B
ATOM	1306	O	SER	179	33.313	26.894	68.860	1.00	52.07	B
ATOM	1307	N	GLU	180	32.917	27.535	66.743	1.00	51.08	B
ATOM	1308	CA	GLU	180	31.467	27.541	66.882	1.00	50.67	B
ATOM	1309	CB	GLU	180	30.834	28.188	65.639	1.00	53.74	B
ATOM	1310	CG	GLU	180	29.322	28.334	65.691	1.00	57.88	B
ATOM	1311	CD	GLU	180	28.872	29.401	66.666	1.00	60.00	B
ATOM	1312	OE1	GLU	180	29.192	29.279	67.868	1.00	61.89	B
ATOM	1313	OE2	GLU	180	28.199	30.362	66.230	1.00	61.08	B
ATOM	1314	C	GLU	180	30.989	26.096	67.026	1.00	48.91	B
ATOM	1315	O	GLU	180	31.307	25.249	66.196	1.00	49.20	B
ATOM	1316	N	ARG	181	30.234	25.817	68.082	1.00	46.31	B
ATOM	1317	CA	ARG	181	29.739	24.472	68.332	1.00	44.31	B
ATOM	1318	CB	ARG	181	30.194	24.018	69.710	1.00	46.69	B
ATOM	1319	CG	ARG	181	29.815	24.962	70.842	1.00	50.74	B
ATOM	1320	CD	ARG	181	28.527	24.530	71.547	1.00	55.78	B
ATOM	1321	NE	ARG	181	28.677	23.242	72.234	1.00	60.23	B
ATOM	1322	CZ	ARG	181	27.708	22.628	72.913	1.00	61.32	B
ATOM	1323	NH1	ARG	181	26.501	23.180	73.007	1.00	61.66	B
ATOM	1324	NH2	ARG	181	27.945	21.453	73.490	1.00	61.67	B
ATOM	1325	C	ARG	181	28.217	24.395	68.211	1.00	42.65	B
ATOM	1326	O	ARG	181	27.491	25.115	68.888	1.00	42.59	B
ATOM	1327	N	LEU	182	27.739	23.510	67.344	1.00	39.35	B

ATOM	1328	CA	LEU	182	26.310	23.355	67.110	1.00	35.22	B	
ATOM	1329	CB	LEU	182	26.088	22.559	65.843	1.00	32.83	B	
ATOM	1330	CG	LEU	182	26.998	22.979	64.710	1.00	31.23	B	
ATOM	1331	CD1	LEU	182	26.730	22.114	63.508	1.00	32.55	B	
ATOM	1332	CD2	LEU	182	26.776	24.444	64.386	1.00	31.45	B	
ATOM	1333	C	LEU	182	25.581	22.690	68.260	1.00	33.98	B	
ATOM	1334	O	LEU	182	26.197	22.057	69.117	1.00	33.33	B	
ATOM	1335	N	GLN	183	24.259	22.843	68.266	1.00	33.26	B	
ATOM	1336	CA	GLN	183	23.399	22.259	69.296	1.00	32.84	B	
ATOM	1337	CB	GLN	183	22.430	23.320	69.842	1.00	34.22	B	
ATOM	1338	CG	GLN	183	23.122	24.542	70.436	1.00	37.39	B	
ATOM	1339	CD	GLN	183	22.163	25.699	70.671	1.00	38.77	B	
ATOM	1340	OE1	GLN	183	21.325	26.003	69.818	1.00	39.62	B	
ATOM	1341	NE2	GLN	183	22.294	26.361	71.820	1.00	37.72	B	
ATOM	1342	C	GLN	183	22.603	21.099	68.706	1.00	31.57	B	
ATOM	1343	O	GLN	183	22.209	21.134	67.545	1.00	31.18	B	
ATOM	1344	N	MET	184	22.353	20.079	69.513	1.00	31.59	B	
ATOM	1345	CA	MET	184	21.622	18.908	69.052	1.00	32.44	B	
ATOM	1346	CB	MET	184	22.480	17.677	69.297	1.00	32.63	B	
ATOM	1347	CG	MET	184	22.018	16.404	68.626	1.00	34.09	B	
ATOM	1348	SD	MET	184	23.162	15.016	68.908	1.00	32.00	B	
ATOM	1349	CE	MET	184	22.574	14.436	70.488	1.00	31.68	B	
ATOM	1350	C	MET	184	20.289	18.787	69.791	1.00	34.68	B	
ATOM	1351	O	MET	184	20.203	19.114	70.976	1.00	35.18	B	
ATOM	1352	N	PHE	185	19.248	18.345	69.086	1.00	36.66	B	
ATOM	1353	CA	PHE	185	17.922	18.168	69.690	1.00	39.01	B	
ATOM	1354	CB	PHE	185	16.987	19.422	69.462	1.00	37.84	B	
ATOM	1355	CG	PHE	185	17.676	20.750	69.619	1.00	38.18	B	
ATOM	1356	CD1	PHE	185	18.453	21.270	68.593	1.00	36.50	B	
ATOM	1357	CD2	PHE	185	17.534	21.488	70.793	1.00	38.31	B	
ATOM	1358	CE1	PHE	185	19.080	22.502	68.724	1.00	36.83	B	
ATOM	1359	CE2	PHE	185	18.158	22.724	70.936	1.00	38.32	B	
ATOM	1360	CZ	PHE	185	18.933	23.232	69.897	1.00	38.06	B	
ATOM	1361	C	PHE	185	17.224	16.956	69.077	1.00	40.70	B	
ATOM	1362	O	PHE	185	17.485	16.598	67.931	1.00	39.58	B	
ATOM	1363	N	ASP	186	16.333	16.330	69.838	1.00	43.77	B	
ATOM	1364	CA	ASP	186	15.588	15.187	69.328	1.00	46.67	B	
ATOM	1365	CB	ASP	186	14.737	14.550	70.419	1.00	47.89	B	
ATOM	1366	CG	ASP	186	15.534	14.206	71.659	1.00	50.45	B	
ATOM	1367	OD1	ASP	186	16.535	13.461	71.540	1.00	50.63	B	
ATOM	1368	OD2	ASP	186	15.154	14.679	72.756	1.00	51.23	B	
ATOM	1369	C	ASP	186	14.668	15.740	68.262	1.00	47.79	B	
ATOM	1370	O	ASP	186	14.371	16.933	68.246	1.00	47.04	B	
ATOM	1371	N	ASP	187	14.215	14.883	67.365	1.00	50.77	B	
ATOM	1372	CA	ASP	187	13.318	15.351	66.328	1.00	54.90	B	
ATOM	1373	CB	ASP	187	13.748	14.832	64.990	1.00	56.93	B	
ATOM	1374	CG	ASP	187	12.973	15.457	63.860	1.00	59.28	B	
ATOM	1375	OD1	ASP	187	13.425	15.343	62.700	1.00	60.01	B	
ATOM	1376	OD2	ASP	187	11.910	16.060	64.138	1.00	60.38	B	
ATOM	1377	C	ASP	187	11.915	14.877	66.662	1.00	56.34	B	
ATOM	1378	O	ASP	187	11.638	13.678	66.649	1.00	56.08	B	
ATOM	1379	N	PRO	188	11.015	15.820	66.985	1.00	58.11	B	
ATOM	1380	CD	PRO	188	11.251	17.274	66.963	1.00	57.99	B	
ATOM	1381	CA	PRO	188	9.621	15.529	67.339	1.00	60.11	B	
ATOM	1382	CB	PRO	188	8.978	16.890	67.309	1.00	59.76	B	
ATOM	1383	CG	PRO	188	10.091	17.790	67.764	1.00	58.23	B	
ATOM	1384	C	PRO	188	8.956	14.549	66.376	1.00	61.87	B	
ATOM	1385	O	PRO	188	8.162	13.700	66.783	1.00	61.46	B	
ATOM	1386	N	ARG	189	9.302	14.669	65.100	1.00	64.31	B	
ATOM	1387	CA	ARG	189	8.757	13.812	64.058	1.00	66.68	B	
ATOM	1388	CB	ARG	189	9.307	14.265	62.701	1.00	66.61	B	
ATOM	1389	CG	ARG	189	8.813	15.651	62.277	1.00	66.58	B	
ATOM	1390	CD	ARG	189	9.586	16.213	61.080	1.00	66.65	B	
ATOM	1391	NE	ARG	189	10.834	16.866	61.474	1.00	66.32	B	
ATOM	1392	CZ	ARG	189	11.704	17.407	60.625	1.00	66.09	B	
ATOM	1393	NH1	ARG	189	11.474	17.377	59.319	1.00	66.33	B	
ATOM	1394	NH2	ARG	189	12.803	17.988	61.083	1.00	65.55	B	
ATOM	1395	C	ARG	189	9.041	12.321	64.289	1.00	68.64	B	
ATOM	1396	O	ARG	189	8.300	11.461	63.813	1.00	69.00	B	
ATOM	1397	N	ASN	190	10.110	12.018	65.022	1.00	71.07	B	
ATOM	1398	CA	ASN	190	10.487	10.634	65.329	1.00	72.28	B	
ATOM	1399	CB	ASN	190	10.758	9.814	63.998	1.00	72.30	B	
ATOM	1400	CG	ASN	190	11.706	10.525	63.041	1.00	71.90	B	

ATOM	1401	OD1	ASN	190	12.847	10.822	63.385	1.00	71.47	B
ATOM	1402	ND2	ASN	190	11.233	10.789	61.826	1.00	71.27	B
ATOM	1403	C	ASN	190	11.709	10.579	66.252	1.00	73.09	B
ATOM	1404	O	ASN	190	12.783	11.067	65.905	1.00	73.71	B
ATOM	1405	N	LYS	191	11.534	9.979	67.427	1.00	73.58	B
ATOM	1406	CA	LYS	191	12.601	9.871	68.428	1.00	73.23	B
ATOM	1407	CB	LYS	191	12.123	9.021	69.606	1.00	75.05	B
ATOM	1408	CG	LYS	191	11.285	9.778	70.614	1.00	76.84	B
ATOM	1409	CD	LYS	191	12.074	10.920	71.241	1.00	77.87	B
ATOM	1410	CE	LYS	191	11.299	11.547	72.387	1.00	78.94	B
ATOM	1411	NZ	LYS	191	9.939	11.988	71.961	1.00	79.06	B
ATOM	1412	C	LYS	191	13.965	9.351	67.968	1.00	71.65	B
ATOM	1413	O	LYS	191	15.000	9.869	68.395	1.00	71.97	B
ATOM	1414	N	ARG	192	13.977	8.326	67.121	1.00	68.70	B
ATOM	1415	CA	ARG	192	15.238	7.772	66.638	1.00	65.72	B
ATOM	1416	CB	ARG	192	14.978	6.515	65.768	1.00	67.67	B
ATOM	1417	CG	ARG	192	16.217	5.978	65.052	1.00	69.51	B
ATOM	1418	CD	ARG	192	16.068	4.519	64.616	1.00	70.83	B
ATOM	1419	NE	ARG	192	14.855	4.261	63.839	1.00	71.87	B
ATOM	1420	CZ	ARG	192	13.672	3.950	64.364	1.00	71.73	B
ATOM	1421	NH1	ARG	192	13.527	3.855	65.681	1.00	70.61	B
ATOM	1422	NH2	ARG	192	12.631	3.727	63.569	1.00	71.53	B
ATOM	1423	C	ARG	192	16.033	8.803	65.843	1.00	62.08	B
ATOM	1424	O	ARG	192	17.190	8.572	65.482	1.00	61.32	B
ATOM	1425	N	GLY	193	15.403	9.946	65.585	1.00	58.42	B
ATOM	1426	CA	GLY	193	16.045	11.008	64.828	1.00	52.07	B
ATOM	1427	C	GLY	193	16.519	12.171	65.674	1.00	47.14	B
ATOM	1428	O	GLY	193	16.159	12.300	66.843	1.00	46.94	B
ATOM	1429	N	VAL	194	17.323	13.033	65.067	1.00	44.16	B
ATOM	1430	CA	VAL	194	17.875	14.184	65.757	1.00	40.67	B
ATOM	1431	CB	VAL	194	19.266	13.838	66.329	1.00	39.96	B
ATOM	1432	CG1	VAL	194	20.338	14.058	65.271	1.00	37.96	B
ATOM	1433	CG2	VAL	194	19.539	14.653	67.564	1.00	39.63	B
ATOM	1434	C	VAL	194	18.008	15.373	64.800	1.00	39.90	B
ATOM	1435	O	VAL	194	18.145	15.194	63.592	1.00	40.91	B
ATOM	1436	N	ILE	195	17.965	16.585	65.347	1.00	38.55	B
ATOM	1437	CA	ILE	195	18.104	17.803	64.553	1.00	35.81	B
ATOM	1438	CB	ILE	195	16.862	18.728	64.709	1.00	38.25	B
ATOM	1439	CG2	ILE	195	17.132	20.092	64.055	1.00	38.19	B
ATOM	1440	CG1	ILE	195	15.615	18.049	64.084	1.00	39.77	B
ATOM	1441	CD1	ILE	195	14.321	18.863	64.185	1.00	41.59	B
ATOM	1442	C	ILE	195	19.347	18.581	65.001	1.00	32.57	B
ATOM	1443	O	ILE	195	19.452	18.970	66.162	1.00	30.74	B
ATOM	1444	N	ILE	196	20.292	18.787	64.086	1.00	29.82	B
ATOM	1445	CA	ILE	196	21.500	19.539	64.405	1.00	27.94	B
ATOM	1446	CB	ILE	196	22.800	18.919	63.769	1.00	26.64	B
ATOM	1447	CG2	ILE	196	24.006	19.816	64.070	1.00	21.22	B
ATOM	1448	CG1	ILE	196	23.110	17.510	64.383	1.00	24.18	B
ATOM	1449	CD1	ILE	196	22.375	16.374	63.764	1.00	22.10	B
ATOM	1450	C	ILE	196	21.303	20.951	63.872	1.00	27.99	B
ATOM	1451	O	ILE	196	21.375	21.196	62.669	1.00	27.68	B
ATOM	1452	N	LYS	197	21.044	21.876	64.784	1.00	29.44	B
ATOM	1453	CA	LYS	197	20.813	23.265	64.426	1.00	30.91	B
ATOM	1454	CB	LYS	197	20.205	24.026	65.616	1.00	33.42	B
ATOM	1455	CG	LYS	197	19.931	25.486	65.303	1.00	35.76	B
ATOM	1456	CD	LYS	197	19.670	26.299	66.548	1.00	39.21	B
ATOM	1457	CE	LYS	197	19.686	27.776	66.199	1.00	42.14	B
ATOM	1458	NZ	LYS	197	20.909	28.121	65.411	1.00	42.07	B
ATOM	1459	C	LYS	197	22.073	23.984	63.971	1.00	29.67	B
ATOM	1460	O	LYS	197	23.080	23.977	64.674	1.00	29.22	B
ATOM	1461	N	GLY	198	22.005	24.600	62.792	1.00	29.85	B
ATOM	1462	CA	GLY	198	23.141	25.345	62.275	1.00	30.66	B
ATOM	1463	C	GLY	198	24.040	24.637	61.282	1.00	30.74	B
ATOM	1464	O	GLY	198	24.857	25.283	60.618	1.00	30.16	B
ATOM	1465	N	LEU	199	23.903	23.318	61.178	1.00	30.32	B
ATOM	1466	CA	LEU	199	24.722	22.538	60.255	1.00	30.74	B
ATOM	1467	CB	LEU	199	24.530	21.004	60.530	1.00	30.24	B
ATOM	1468	CG	LEU	199	25.328	19.967	59.664	1.00	28.88	B
ATOM	1469	CD1	LEU	199	26.773	20.398	59.527	1.00	30.22	B
ATOM	1470	CD2	LEU	199	25.254	18.587	60.308	1.00	28.26	B
ATOM	1471	C	LEU	199	24.397	22.869	58.792	1.00	31.25	B
ATOM	1472	O	LEU	199	23.256	22.699	58.340	1.00	31.36	B
ATOM	1473	N	GLU	200	25.406	23.345	58.065	1.00	30.26	B

ATOM	1474	CA	GLU	200	25.253	23.712	56.661	1.00	32.06	B
ATOM	1475	CB	GLU	200	26.446	24.590	56.190	1.00	34.38	B
ATOM	1476	CG	GLU	200	26.604	25.870	56.961	1.00	41.33	B
ATOM	1477	CD	GLU	200	25.395	26.773	56.833	1.00	42.76	B
ATOM	1478	OE1	GLU	200	25.121	27.535	57.785	1.00	43.19	B
ATOM	1479	OE2	GLU	200	24.730	26.721	55.776	1.00	43.56	B
ATOM	1480	C	GLU	200	25.164	22.514	55.722	1.00	31.83	B
ATOM	1481	O	GLU	200	25.841	21.503	55.916	1.00	30.83	B
ATOM	1482	N	GLU	201	24.328	22.654	54.700	1.00	30.84	B
ATOM	1483	CA	GLU	201	24.163	21.639	53.677	1.00	30.37	B
ATOM	1484	CB	GLU	201	22.732	21.167	53.611	1.00	30.91	B
ATOM	1485	CG	GLU	201	22.386	20.111	54.629	1.00	33.83	B
ATOM	1486	CD	GLU	201	20.975	19.587	54.454	1.00	36.02	B
ATOM	1487	OE1	GLU	201	20.052	20.163	55.069	1.00	37.16	B
ATOM	1488	OE2	GLU	201	20.791	18.604	53.695	1.00	36.56	B
ATOM	1489	C	GLU	201	24.528	22.328	52.373	1.00	30.44	B
ATOM	1490	O	GLU	201	23.796	23.207	51.919	1.00	30.69	B
ATOM	1491	N	ILE	202	25.663	21.958	51.783	1.00	28.80	B
ATOM	1492	CA	ILE	202	26.073	22.575	50.526	1.00	28.82	B
ATOM	1493	CB	ILE	202	27.619	22.739	50.409	1.00	28.91	B
ATOM	1494	CG2	ILE	202	27.978	23.225	49.014	1.00	26.00	B
ATOM	1495	CG1	ILE	202	28.137	23.751	51.426	1.00	28.90	B
ATOM	1496	CD1	ILE	202	28.057	23.294	52.863	1.00	32.03	B
ATOM	1497	C	ILE	202	25.594	21.773	49.324	1.00	28.57	B
ATOM	1498	O	ILE	202	25.844	20.571	49.215	1.00	29.93	B
ATOM	1499	N	THR	203	24.896	22.448	48.422	1.00	28.23	B
ATOM	1500	CA	THR	203	24.404	21.803	47.219	1.00	26.49	B
ATOM	1501	CB	THR	203	23.307	22.665	46.527	1.00	26.14	B
ATOM	1502	OG1	THR	203	22.173	22.791	47.401	1.00	24.25	B
ATOM	1503	CG2	THR	203	22.862	22.028	45.208	1.00	25.01	B
ATOM	1504	C	THR	203	25.606	21.636	46.293	1.00	26.13	B
ATOM	1505	O	THR	203	26.483	22.495	46.253	1.00	26.91	B
ATOM	1506	N	VAL	204	25.666	20.504	45.599	1.00	26.49	B
ATOM	1507	CA	VAL	204	26.741	20.220	44.654	1.00	27.51	B
ATOM	1508	CB	VAL	204	27.444	18.868	44.967	1.00	25.76	B
ATOM	1509	CG1	VAL	204	28.653	18.672	44.056	1.00	23.12	B
ATOM	1510	CG2	VAL	204	27.879	18.837	46.423	1.00	24.79	B
ATOM	1511	C	VAL	204	26.009	20.149	43.321	1.00	29.14	B
ATOM	1512	O	VAL	204	25.265	19.199	43.061	1.00	30.39	B
ATOM	1513	N	HIS	205	26.218	21.170	42.495	1.00	29.22	B
ATOM	1514	CA	HIS	205	25.553	21.313	41.195	1.00	30.55	B
ATOM	1515	CB	HIS	205	25.613	22.794	40.767	1.00	28.34	B
ATOM	1516	CG	HIS	205	25.157	23.732	41.838	1.00	28.46	B
ATOM	1517	CD2	HIS	205	25.858	24.492	42.711	1.00	27.43	B
ATOM	1518	ND1	HIS	205	23.832	23.862	42.196	1.00	28.83	B
ATOM	1519	CE1	HIS	205	23.736	24.654	43.249	1.00	28.44	B
ATOM	1520	NE2	HIS	205	24.952	25.049	43.582	1.00	29.92	B
ATOM	1521	C	HIS	205	26.092	20.435	40.081	1.00	31.51	B
ATOM	1522	O	HIS	205	25.358	20.055	39.169	1.00	31.34	B
ATOM	1523	N	ASN	206	27.383	20.136	40.147	1.00	33.49	B
ATOM	1524	CA	ASN	206	28.032	19.299	39.151	1.00	34.62	B
ATOM	1525	CB	ASN	206	28.444	20.138	37.930	1.00	34.75	B
ATOM	1526	CG	ASN	206	29.164	21.417	38.309	1.00	35.27	B
ATOM	1527	OD1	ASN	206	30.224	21.391	38.938	1.00	37.58	B
ATOM	1528	ND2	ASN	206	28.589	22.548	37.925	1.00	34.11	B
ATOM	1529	C	ASN	206	29.243	18.650	39.798	1.00	35.69	B
ATOM	1530	O	ASN	206	29.478	18.836	40.992	1.00	36.45	B
ATOM	1531	N	LYS	207	30.002	17.876	39.031	1.00	36.43	B
ATOM	1532	CA	LYS	207	31.171	17.216	39.590	1.00	38.62	B
ATOM	1533	CB	LYS	207	31.582	15.993	38.703	1.00	40.10	B
ATOM	1534	CG	LYS	207	32.123	16.339	37.319	1.00	42.56	B
ATOM	1535	CD	LYS	207	32.259	15.081	36.456	1.00	44.26	B
ATOM	1536	CE	LYS	207	33.191	15.293	35.267	1.00	43.78	B
ATOM	1537	NZ	LYS	207	34.613	15.454	35.696	1.00	42.46	B
ATOM	1538	C	LYS	207	32.313	18.222	39.700	1.00	39.03	B
ATOM	1539	O	LYS	207	33.176	18.120	40.576	1.00	38.73	B
ATOM	1540	N	ASP	208	32.292	19.208	38.813	1.00	39.88	B
ATOM	1541	CA	ASP	208	33.312	20.244	38.790	1.00	40.76	B
ATOM	1542	CB	ASP	208	33.248	20.981	37.461	1.00	42.58	B
ATOM	1543	CG	ASP	208	33.659	20.101	36.292	1.00	45.91	B
ATOM	1544	OD1	ASP	208	33.407	20.484	35.127	1.00	46.74	B
ATOM	1545	OD2	ASP	208	34.246	19.023	36.542	1.00	46.78	B
ATOM	1546	C	ASP	208	33.141	21.219	39.952	1.00	39.55	B

ATOM	1547	O	ASP	208	33.643	22.339	39.922	1.00	41.22	B
ATOM	1548	N	GLU	209	32.457	20.784	40.996	1.00	37.46	B
ATOM	1549	CA	GLU	209	32.241	21.660	42.128	1.00	35.89	B
ATOM	1550	CB	GLU	209	30.760	22.075	42.158	1.00	35.84	B
ATOM	1551	CG	GLU	209	30.445	23.275	43.010	1.00	37.17	B
ATOM	1552	CD	GLU	209	28.973	23.682	42.924	1.00	38.94	B
ATOM	1553	OE1	GLU	209	28.462	23.857	41.793	1.00	37.72	B
ATOM	1554	OE2	GLU	209	28.327	23.835	43.988	1.00	38.77	B
ATOM	1555	C	GLU	209	32.646	20.992	43.439	1.00	34.61	B
ATOM	1556	O	GLU	209	32.763	21.657	44.470	1.00	36.51	B
ATOM	1557	N	VAL	210	32.907	19.690	43.395	1.00	32.07	B
ATOM	1558	CA	VAL	210	33.268	18.966	44.609	1.00	29.92	B
ATOM	1559	CB	VAL	210	33.065	17.411	44.450	1.00	29.01	B
ATOM	1560	CG1	VAL	210	31.856	17.110	43.574	1.00	26.09	B
ATOM	1561	CG2	VAL	210	34.301	16.774	43.901	1.00	29.03	B
ATOM	1562	C	VAL	210	34.668	19.212	45.183	1.00	28.45	B
ATOM	1563	O	VAL	210	34.820	19.322	46.406	1.00	29.31	B
ATOM	1564	N	TYR	211	35.694	19.311	44.343	1.00	26.40	B
ATOM	1565	CA	TYR	211	37.038	19.505	44.894	1.00	24.93	B
ATOM	1566	CB	TYR	211	38.106	19.552	43.783	1.00	22.02	B
ATOM	1567	CG	TYR	211	39.510	19.386	44.318	1.00	23.83	B
ATOM	1568	CD1	TYR	211	39.850	18.284	45.097	1.00	26.06	B
ATOM	1569	CE1	TYR	211	41.136	18.131	45.625	1.00	25.76	B
ATOM	1570	CD2	TYR	211	40.498	20.339	44.074	1.00	24.90	B
ATOM	1571	CE2	TYR	211	41.790	20.196	44.597	1.00	24.81	B
ATOM	1572	CZ	TYR	211	42.103	19.089	45.374	1.00	25.75	B
ATOM	1573	OH	TYR	211	43.373	18.938	45.910	1.00	23.97	B
ATOM	1574	C	TYR	211	37.111	20.759	45.757	1.00	25.45	B
ATOM	1575	O	TYR	211	37.691	20.740	46.844	1.00	24.21	B
ATOM	1576	N	GLN	212	36.501	21.840	45.272	1.00	27.99	B
ATOM	1577	CA	GLN	212	36.473	23.117	45.983	1.00	27.45	B
ATOM	1578	CB	GLN	212	35.721	24.126	45.163	1.00	31.66	B
ATOM	1579	CG	GLN	212	35.365	25.402	45.907	1.00	37.63	B
ATOM	1580	CD	GLN	212	35.696	26.654	45.105	1.00	40.53	B
ATOM	1581	OE1	GLN	212	35.305	26.782	43.937	1.00	39.59	B
ATOM	1582	NE2	GLN	212	36.418	27.587	45.731	1.00	39.73	B
ATOM	1583	C	GLN	212	35.834	22.981	47.364	1.00	26.73	B
ATOM	1584	O	GLN	212	36.329	23.527	48.347	1.00	26.01	B
ATOM	1585	N	ILE	213	34.733	22.243	47.437	1.00	26.10	B
ATOM	1586	CA	ILE	213	34.044	22.037	48.703	1.00	24.91	B
ATOM	1587	CB	ILE	213	32.694	21.327	48.496	1.00	23.51	B
ATOM	1588	CG2	ILE	213	31.978	21.200	49.835	1.00	20.39	B
ATOM	1589	CG1	ILE	213	31.843	22.117	47.461	1.00	22.89	B
ATOM	1590	CD1	ILE	213	30.472	21.509	47.152	1.00	23.13	B
ATOM	1591	C	ILE	213	34.906	21.207	49.656	1.00	25.49	B
ATOM	1592	O	ILE	213	34.916	21.448	50.865	1.00	24.30	B
ATOM	1593	N	LEU	214	35.618	20.226	49.106	1.00	26.92	B
ATOM	1594	CA	LEU	214	36.496	19.381	49.905	1.00	28.08	B
ATOM	1595	CB	LEU	214	37.031	18.168	49.050	1.00	28.21	B
ATOM	1596	CG	LEU	214	36.272	16.802	49.152	1.00	30.13	B
ATOM	1597	CD1	LEU	214	34.796	17.034	49.411	1.00	31.20	B
ATOM	1598	CD2	LEU	214	36.482	15.987	47.876	1.00	29.12	B
ATOM	1599	C	LEU	214	37.657	20.225	50.442	1.00	29.28	B
ATOM	1600	O	LEU	214	38.012	20.114	51.620	1.00	30.45	B
ATOM	1601	N	GLU	215	38.235	21.083	49.599	1.00	28.08	B
ATOM	1602	CA	GLU	215	39.339	21.932	50.059	1.00	28.89	B
ATOM	1603	CB	GLU	215	39.864	22.842	48.914	1.00	29.69	B
ATOM	1604	CG	GLU	215	40.426	22.093	47.714	1.00	33.51	B
ATOM	1605	CD	GLU	215	41.092	23.014	46.700	1.00	36.27	B
ATOM	1606	OE1	GLU	215	42.343	23.136	46.730	1.00	34.34	B
ATOM	1607	OE2	GLU	215	40.358	23.620	45.880	1.00	36.57	B
ATOM	1608	C	GLU	215	38.919	22.795	51.255	1.00	28.03	B
ATOM	1609	O	GLU	215	39.682	22.953	52.210	1.00	27.31	B
ATOM	1610	N	LYS	216	37.707	23.348	51.204	1.00	27.99	B
ATOM	1611	CA	LYS	216	37.202	24.183	52.290	1.00	29.52	B
ATOM	1612	CB	LYS	216	35.799	24.696	51.971	1.00	30.11	B
ATOM	1613	CG	LYS	216	35.691	25.416	50.650	1.00	32.53	B
ATOM	1614	CD	LYS	216	36.584	26.643	50.602	1.00	34.31	B
ATOM	1615	CE	LYS	216	36.596	27.272	49.200	1.00	36.64	B
ATOM	1616	NZ	LYS	216	37.248	26.419	48.152	1.00	34.44	B
ATOM	1617	C	LYS	216	37.170	23.415	53.609	1.00	30.05	B
ATOM	1618	O	LYS	216	37.516	23.960	54.658	1.00	31.96	B
ATOM	1619	N	GLY	217	36.742	22.156	53.553	1.00	30.83	B

ATOM	1620	CA	GLY	217	36.695	21.335	54.752	1.00	29.82	B
ATOM	1621	C	GLY	217	38.107	21.144	55.270	1.00	29.77	B
ATOM	1622	O	GLY	217	38.389	21.354	56.460	1.00	28.73	B
ATOM	1623	N	ALA	218	39.000	20.749	54.363	1.00	29.20	B
ATOM	1624	CA	ALA	218	40.404	20.548	54.696	1.00	28.09	B
ATOM	1625	CB	ALA	218	41.212	20.299	53.427	1.00	25.39	B
ATOM	1626	C	ALA	218	40.924	21.792	55.422	1.00	27.61	B
ATOM	1627	O	ALA	218	41.623	21.684	56.429	1.00	27.17	B
ATOM	1628	N	ALA	219	40.559	22.969	54.914	1.00	27.54	B
ATOM	1629	CA	ALA	219	40.984	24.243	55.505	1.00	27.45	B
ATOM	1630	CB	ALA	219	40.430	25.406	54.695	1.00	26.20	B
ATOM	1631	C	ALA	219	40.553	24.385	56.964	1.00	27.16	B
ATOM	1632	O	ALA	219	41.368	24.726	57.833	1.00	26.05	B
ATOM	1633	N	LYS	220	39.273	24.135	57.227	1.00	26.17	B
ATOM	1634	CA	LYS	220	38.754	24.234	58.585	1.00	26.59	B
ATOM	1635	CB	LYS	220	37.203	24.057	58.592	1.00	25.82	B
ATOM	1636	CG	LYS	220	36.477	25.037	57.691	1.00	26.36	B
ATOM	1637	CD	LYS	220	34.997	25.195	58.065	1.00	28.61	B
ATOM	1638	CE	LYS	220	34.827	25.771	59.471	1.00	27.13	B
ATOM	1639	NZ	LYS	220	33.406	26.129	59.789	1.00	25.98	B
ATOM	1640	C	LYS	220	39.426	23.190	59.491	1.00	26.00	B
ATOM	1641	O	LYS	220	39.715	23.465	60.665	1.00	24.88	B
ATOM	1642	N	ARG	221	39.671	22.000	58.937	1.00	24.80	B
ATOM	1643	CA	ARG	221	40.330	20.916	59.671	1.00	22.73	B
ATOM	1644	CB	ARG	221	40.685	19.757	58.725	1.00	24.70	B
ATOM	1645	CG	ARG	221	39.524	18.885	58.293	1.00	25.62	B
ATOM	1646	CD	ARG	221	39.367	17.736	59.256	1.00	26.10	B
ATOM	1647	NE	ARG	221	38.190	16.934	58.960	1.00	24.76	B
ATOM	1648	CZ	ARG	221	38.065	16.146	57.901	1.00	22.87	B
ATOM	1649	NH1	ARG	221	39.061	16.051	57.021	1.00	19.50	B
ATOM	1650	NH2	ARG	221	36.942	15.451	57.735	1.00	20.09	B
ATOM	1651	C	ARG	221	41.624	21.456	60.267	1.00	21.95	B
ATOM	1652	O	ARG	221	41.889	21.306	61.466	1.00	20.88	B
ATOM	1653	N	THR	222	42.421	22.089	59.406	1.00	20.21	B
ATOM	1654	CA	THR	222	43.705	22.661	59.795	1.00	19.39	B
ATOM	1655	CB	THR	222	44.312	23.464	58.650	1.00	21.09	B
ATOM	1656	OG1	THR	222	44.502	22.600	57.525	1.00	22.38	B
ATOM	1657	CG2	THR	222	45.649	24.077	59.073	1.00	20.44	B
ATOM	1658	C	THR	222	43.589	23.579	60.991	1.00	18.28	B
ATOM	1659	O	THR	222	44.338	23.441	61.952	1.00	17.80	B
ATOM	1660	N	THR	223	42.649	24.517	60.926	1.00	17.37	B
ATOM	1661	CA	THR	223	42.452	25.461	62.012	1.00	18.66	B
ATOM	1662	CB	THR	223	41.496	26.590	61.605	1.00	17.71	B
ATOM	1663	OG1	THR	223	40.245	26.413	62.268	1.00	20.08	B
ATOM	1664	CG2	THR	223	41.258	26.581	60.111	1.00	16.54	B
ATOM	1665	C	THR	223	41.902	24.740	63.242	1.00	20.76	B
ATOM	1666	O	THR	223	42.206	25.120	64.374	1.00	24.08	B
ATOM	1667	N	ALA	224	41.100	23.698	63.018	1.00	21.47	B
ATOM	1668	CA	ALA	224	40.529	22.898	64.105	1.00	19.87	B
ATOM	1669	CB	ALA	224	39.642	21.801	63.534	1.00	22.14	B
ATOM	1670	C	ALA	224	41.667	22.266	64.894	1.00	19.87	B
ATOM	1671	O	ALA	224	41.689	22.289	66.129	1.00	16.71	B
ATOM	1672	N	ALA	225	42.604	21.680	64.155	1.00	20.37	B
ATOM	1673	CA	ALA	225	43.765	21.048	64.755	1.00	20.88	B
ATOM	1674	CB	ALA	225	44.647	20.440	63.666	1.00	19.50	B
ATOM	1675	C	ALA	225	44.541	22.096	65.553	1.00	22.18	B
ATOM	1676	O	ALA	225	45.054	21.808	66.638	1.00	20.94	B
ATOM	1677	N	THR	226	44.613	23.319	65.023	1.00	23.92	B
ATOM	1678	CA	THR	226	45.324	24.401	65.717	1.00	24.83	B
ATOM	1679	CB	THR	226	45.313	25.723	64.895	1.00	24.59	B
ATOM	1680	OG1	THR	226	46.088	25.565	63.699	1.00	23.18	B
ATOM	1681	CG2	THR	226	45.904	26.866	65.721	1.00	25.23	B
ATOM	1682	C	THR	226	44.699	24.679	67.089	1.00	25.41	B
ATOM	1683	O	THR	226	45.405	24.877	68.083	1.00	25.12	B
ATOM	1684	N	LEU	227	43.370	24.680	67.130	1.00	25.47	B
ATOM	1685	CA	LEU	227	42.619	24.942	68.353	1.00	26.90	B
ATOM	1686	CB	LEU	227	41.222	25.541	67.980	1.00	29.00	B
ATOM	1687	CG	LEU	227	41.051	27.041	67.561	1.00	32.68	B
ATOM	1688	CD1	LEU	227	42.240	27.567	66.763	1.00	31.51	B
ATOM	1689	CD2	LEU	227	39.756	27.156	66.755	1.00	32.75	B
ATOM	1690	C	LEU	227	42.409	23.739	69.296	1.00	26.44	B
ATOM	1691	O	LEU	227	42.348	23.906	70.520	1.00	25.50	B
ATOM	1692	N	MET	228	42.295	22.533	68.755	1.00	24.99	B

ATOM	1693	CA	MET	228	42.041	21.392	69.635	1.00	25.58	B
ATOM	1694	CB	MET	228	40.625	20.786	69.310	1.00	27.00	B
ATOM	1695	CG	MET	228	39.499	21.798	69.554	1.00	28.30	B
ATOM	1696	SD	MET	228	37.874	21.368	68.919	1.00	31.74	B
ATOM	1697	CE	MET	228	37.998	22.026	67.265	1.00	30.21	B
ATOM	1698	C	MET	228	43.091	20.301	69.666	1.00	23.55	B
ATOM	1699	O	MET	228	43.547	19.828	68.629	1.00	23.83	B
ATOM	1700	N	ASN	229	43.471	19.913	70.882	1.00	22.85	B
ATOM	1701	CA	ASN	229	44.470	18.870	71.099	1.00	21.02	B
ATOM	1702	CB	ASN	229	44.574	18.524	72.588	1.00	19.32	B
ATOM	1703	CG	ASN	229	45.172	19.646	73.426	1.00	19.33	B
ATOM	1704	OD1	ASN	229	45.690	20.634	72.899	1.00	19.44	B
ATOM	1705	ND2	ASN	229	45.112	19.484	74.751	1.00	13.92	B
ATOM	1706	C	ASN	229	44.162	17.582	70.329	1.00	21.09	B
ATOM	1707	O	ASN	229	43.063	17.026	70.435	1.00	21.09	B
ATOM	1708	N	ALA	230	45.144	17.121	69.558	1.00	20.25	B
ATOM	1709	CA	ALA	230	45.030	15.887	68.786	1.00	19.42	B
ATOM	1710	CB	ALA	230	45.224	14.675	69.721	1.00	21.67	B
ATOM	1711	C	ALA	230	43.694	15.783	68.067	1.00	18.26	B
ATOM	1712	O	ALA	230	43.096	14.712	68.000	1.00	17.83	B
ATOM	1713	N	TYR	231	43.242	16.897	67.512	1.00	17.17	B
ATOM	1714	CA	TYR	231	41.965	16.927	66.821	1.00	17.72	B
ATOM	1715	CB	TYR	231	41.694	18.379	66.201	1.00	15.95	B
ATOM	1716	CG	TYR	231	40.341	18.465	65.524	1.00	12.55	B
ATOM	1717	CD1	TYR	231	40.205	18.269	64.151	1.00	12.28	B
ATOM	1718	CE1	TYR	231	38.933	18.219	63.555	1.00	8.18	B
ATOM	1719	CD2	TYR	231	39.182	18.621	66.279	1.00	10.61	B
ATOM	1720	CE2	TYR	231	37.918	18.573	65.690	1.00	9.26	B
ATOM	1721	CZ	TYR	231	37.802	18.372	64.338	1.00	6.19	B
ATOM	1722	OH	TYR	231	36.545	18.335	63.777	1.00	8.98	B
ATOM	1723	C	TYR	231	41.728	15.869	65.731	1.00	18.14	B
ATOM	1724	O	TYR	231	40.596	15.392	65.571	1.00	17.92	B
ATOM	1725	N	SER	232	42.769	15.504	64.982	1.00	17.34	B
ATOM	1726	CA	SER	232	42.585	14.537	63.903	1.00	17.96	B
ATOM	1727	CB	SER	232	43.681	14.688	62.816	1.00	13.72	B
ATOM	1728	OG	SER	232	44.941	14.251	63.275	1.00	15.73	B
ATOM	1729	C	SER	232	42.502	13.070	64.323	1.00	18.78	B
ATOM	1730	O	SER	232	41.934	12.255	63.598	1.00	19.24	B
ATOM	1731	N	SER	233	43.051	12.726	65.480	1.00	17.77	B
ATOM	1732	CA	SER	233	43.019	11.340	65.904	1.00	16.56	B
ATOM	1733	CB	SER	233	44.383	10.932	66.496	1.00	18.00	B
ATOM	1734	OG	SER	233	44.509	11.362	67.846	1.00	17.89	B
ATOM	1735	C	SER	233	41.935	11.141	66.943	1.00	17.20	B
ATOM	1736	O	SER	233	41.413	10.035	67.110	1.00	13.55	B
ATOM	1737	N	ARG	234	41.570	12.235	67.609	1.00	18.37	B
ATOM	1738	CA	ARG	234	40.579	12.185	68.678	1.00	18.14	B
ATOM	1739	CB	ARG	234	41.035	13.079	69.848	1.00	20.04	B
ATOM	1740	CG	ARG	234	41.136	12.352	71.169	1.00	23.36	B
ATOM	1741	CD	ARG	234	42.547	12.392	71.767	1.00	25.39	B
ATOM	1742	NE	ARG	234	42.847	13.651	72.455	1.00	28.46	B
ATOM	1743	CZ	ARG	234	43.898	13.844	73.255	1.00	28.83	B
ATOM	1744	NH1	ARG	234	44.765	12.865	73.479	1.00	28.24	B
ATOM	1745	NH2	ARG	234	44.082	15.019	73.842	1.00	28.56	B
ATOM	1746	C	ARG	234	39.142	12.524	68.318	1.00	17.12	B
ATOM	1747	O	ARG	234	38.262	12.440	69.174	1.00	16.45	B
ATOM	1748	N	SER	235	38.879	12.876	67.064	1.00	17.25	B
ATOM	1749	CA	SER	235	37.508	13.232	66.685	1.00	17.01	B
ATOM	1750	CB	SER	235	37.470	14.581	66.108	1.00	16.15	B
ATOM	1751	OG	SER	235	38.109	14.594	64.847	1.00	15.24	B
ATOM	1752	C	SER	235	36.847	12.297	65.697	1.00	17.23	B
ATOM	1753	O	SER	235	37.505	11.536	64.991	1.00	17.87	B
ATOM	1754	N	HIS	236	35.527	12.381	65.655	1.00	16.90	B
ATOM	1755	CA	HIS	236	34.720	11.580	64.750	1.00	18.47	B
ATOM	1756	CB	HIS	236	33.553	10.961	65.484	1.00	20.05	B
ATOM	1757	CG	HIS	236	33.941	10.192	66.705	1.00	21.39	B
ATOM	1758	CD2	HIS	236	33.907	10.529	68.016	1.00	20.87	B
ATOM	1759	ND1	HIS	236	34.444	8.910	66.650	1.00	21.00	B
ATOM	1760	CE1	HIS	236	34.700	8.490	67.876	1.00	20.80	B
ATOM	1761	NE2	HIS	236	34.385	9.454	68.723	1.00	19.15	B
ATOM	1762	C	HIS	236	34.166	12.518	63.688	1.00	19.93	B
ATOM	1763	O	HIS	236	33.598	13.569	64.005	1.00	18.38	B
ATOM	1764	N	SER	237	34.326	12.155	62.425	1.00	20.64	B
ATOM	1765	CA	SER	237	33.795	13.001	61.374	1.00	21.44	B

ATOM	1766	CB	SER	237	34.889	13.424	60.424	1.00	20.37	B
ATOM	1767	OG	SER	237	35.258	12.370	59.566	1.00	19.17	B
ATOM	1768	C	SER	237	32.731	12.224	60.619	1.00	21.91	B
ATOM	1769	O	SER	237	32.908	11.043	60.320	1.00	21.18	B
ATOM	1770	N	VAL	238	31.620	12.886	60.324	1.00	21.76	B
ATOM	1771	CA	VAL	238	30.548	12.246	59.587	1.00	22.83	B
ATOM	1772	CB	VAL	238	29.297	12.024	60.475	1.00	25.08	B
ATOM	1773	CG1	VAL	238	29.043	13.241	61.323	1.00	27.25	B
ATOM	1774	CG2	VAL	238	28.077	11.717	59.601	1.00	24.91	B
ATOM	1775	C	VAL	238	30.176	13.052	58.366	1.00	21.64	B
ATOM	1776	O	VAL	238	29.399	13.986	58.450	1.00	24.16	B
ATOM	1777	N	PHE	239	30.764	12.683	57.232	1.00	23.48	B
ATOM	1778	CA	PHE	239	30.513	13.331	55.943	1.00	23.45	B
ATOM	1779	CB	PHE	239	31.736	13.139	55.002	1.00	22.63	B
ATOM	1780	CG	PHE	239	31.658	13.923	53.722	1.00	20.75	B
ATOM	1781	CD1	PHE	239	30.660	13.667	52.785	1.00	19.42	B
ATOM	1782	CD2	PHE	239	32.580	14.928	53.458	1.00	20.63	B
ATOM	1783	CE1	PHE	239	30.578	14.403	51.596	1.00	21.05	B
ATOM	1784	CE2	PHE	239	32.510	15.676	52.268	1.00	21.14	B
ATOM	1785	CZ	PHE	239	31.506	15.413	51.334	1.00	19.84	B
ATOM	1786	C	PHE	239	29.286	12.669	55.321	1.00	24.62	B
ATOM	1787	O	PHE	239	29.326	11.482	54.983	1.00	24.57	B
ATOM	1788	N	SER	240	28.202	13.430	55.178	1.00	24.38	B
ATOM	1789	CA	SER	240	26.968	12.910	54.596	1.00	23.26	B
ATOM	1790	CB	SER	240	25.778	13.249	55.480	1.00	22.32	B
ATOM	1791	OG	SER	240	25.932	12.724	56.786	1.00	21.48	B
ATOM	1792	C	SER	240	26.704	13.447	53.199	1.00	23.92	B
ATOM	1793	O	SER	240	27.065	14.568	52.865	1.00	23.73	B
ATOM	1794	N	VAL	241	26.067	12.622	52.382	1.00	25.40	B
ATOM	1795	CA	VAL	241	25.712	12.995	51.022	1.00	25.45	B
ATOM	1796	CB	VAL	241	26.654	12.349	49.985	1.00	26.85	B
ATOM	1797	CG1	VAL	241	26.790	10.856	50.249	1.00	26.88	B
ATOM	1798	CG2	VAL	241	26.118	12.595	48.579	1.00	26.95	B
ATOM	1799	C	VAL	241	24.293	12.513	50.787	1.00	25.56	B
ATOM	1800	O	VAL	241	24.013	11.321	50.856	1.00	25.33	B
ATOM	1801	N	THR	242	23.391	13.454	50.536	1.00	26.85	B
ATOM	1802	CA	THR	242	21.996	13.130	50.302	1.00	26.02	B
ATOM	1803	CB	THR	242	21.091	13.997	51.182	1.00	26.36	B
ATOM	1804	OG1	THR	242	21.447	13.814	52.557	1.00	26.94	B
ATOM	1805	CG2	THR	242	19.628	13.612	50.995	1.00	28.00	B
ATOM	1806	C	THR	242	21.656	13.352	48.832	1.00	27.35	B
ATOM	1807	O	THR	242	22.126	14.311	48.217	1.00	26.21	B
ATOM	1808	N	ILE	243	20.857	12.451	48.263	1.00	28.40	B
ATOM	1809	CA	ILE	243	20.468	12.564	46.861	1.00	28.65	B
ATOM	1810	CB	ILE	243	21.048	11.407	46.017	1.00	28.29	B
ATOM	1811	CG2	ILE	243	20.944	11.746	44.534	1.00	27.94	B
ATOM	1812	CG1	ILE	243	22.526	11.156	46.392	1.00	29.06	B
ATOM	1813	CD1	ILE	243	23.191	10.046	45.592	1.00	25.36	B
ATOM	1814	C	ILE	243	18.950	12.538	46.721	1.00	29.68	B
ATOM	1815	O	ILE	243	18.327	11.512	46.966	1.00	30.63	B
ATOM	1816	N	HIS	244	18.355	13.672	46.358	1.00	31.77	B
ATOM	1817	CA	HIS	244	16.908	13.744	46.158	1.00	32.56	B
ATOM	1818	CB	HIS	244	16.354	15.175	46.421	1.00	33.70	B
ATOM	1819	CG	HIS	244	16.323	15.570	47.864	1.00	34.78	B
ATOM	1820	CD2	HIS	244	15.331	15.500	48.785	1.00	35.77	B
ATOM	1821	ND1	HIS	244	17.405	16.132	48.511	1.00	36.48	B
ATOM	1822	CE1	HIS	244	17.080	16.392	49.765	1.00	35.67	B
ATOM	1823	NE2	HIS	244	15.827	16.018	49.958	1.00	35.06	B
ATOM	1824	C	HIS	244	16.700	13.383	44.693	1.00	33.70	B
ATOM	1825	O	HIS	244	17.271	14.020	43.798	1.00	33.29	B
ATOM	1826	N	MET	245	15.885	12.366	44.448	1.00	34.30	B
ATOM	1827	CA	MET	245	15.654	11.910	43.087	1.00	34.70	B
ATOM	1828	CB	MET	245	16.212	10.483	42.944	1.00	34.85	B
ATOM	1829	CG	MET	245	17.734	10.441	43.100	1.00	35.80	B
ATOM	1830	SD	MET	245	18.439	8.805	43.321	1.00	36.13	B
ATOM	1831	CE	MET	245	18.009	8.537	45.032	1.00	32.87	B
ATOM	1832	C	MET	245	14.203	11.985	42.628	1.00	34.49	B
ATOM	1833	O	MET	245	13.272	11.757	43.402	1.00	33.49	B
ATOM	1834	N	LYS	246	14.026	12.313	41.352	1.00	35.05	B
ATOM	1835	CA	LYS	246	12.700	12.449	40.769	1.00	36.99	B
ATOM	1836	CB	LYS	246	12.280	13.947	40.750	1.00	38.69	B
ATOM	1837	CG	LYS	246	10.919	14.227	40.117	1.00	43.46	B
ATOM	1838	CD	LYS	246	10.702	15.729	39.856	1.00	45.60	B

ATOM	1839	CE	LYS	246	10.795	16.556	41.148	1.00	48.45	B
ATOM	1840	NZ	LYS	246	10.619	18.031	40.940	1.00	46.59	B
ATOM	1841	C	LYS	246	12.654	11.889	39.353	1.00	36.70	B
ATOM	1842	O	LYS	246	13.324	12.387	38.452	1.00	36.63	B
ATOM	1843	N	GLU	247	11.864	10.841	39.166	1.00	36.80	B
ATOM	1844	CA	GLU	247	11.706	10.240	37.854	1.00	37.12	B
ATOM	1845	CB	GLU	247	12.209	8.806	37.866	1.00	37.24	B
ATOM	1846	CG	GLU	247	11.710	7.990	39.036	1.00	37.73	B
ATOM	1847	CD	GLU	247	12.621	6.820	39.347	1.00	38.20	B
ATOM	1848	OE1	GLU	247	12.293	6.035	40.262	1.00	37.07	B
ATOM	1849	OE2	GLU	247	13.670	6.692	38.677	1.00	38.76	B
ATOM	1850	C	GLU	247	10.228	10.299	37.498	1.00	36.40	B
ATOM	1851	O	GLU	247	9.369	10.193	38.365	1.00	35.41	B
ATOM	1852	N	THR	248	9.940	10.498	36.219	1.00	37.67	B
ATOM	1853	CA	THR	248	8.563	10.587	35.746	1.00	39.02	B
ATOM	1854	CB	THR	248	8.344	11.889	34.920	1.00	39.40	B
ATOM	1855	OG1	THR	248	8.754	13.025	35.693	1.00	40.65	B
ATOM	1856	CG2	THR	248	6.877	12.050	34.543	1.00	40.08	B
ATOM	1857	C	THR	248	8.240	9.381	34.863	1.00	39.45	B
ATOM	1858	O	THR	248	8.959	9.095	33.902	1.00	39.20	B
ATOM	1859	N	THR	249	7.158	8.678	35.187	1.00	39.85	B
ATOM	1860	CA	THR	249	6.751	7.515	34.407	1.00	40.93	B
ATOM	1861	CB	THR	249	5.642	6.728	35.119	1.00	41.31	B
ATOM	1862	OG1	THR	249	4.458	7.531	35.190	1.00	40.33	B
ATOM	1863	CG2	THR	249	6.078	6.345	36.527	1.00	39.92	B
ATOM	1864	C	THR	249	6.233	7.952	33.039	1.00	41.94	B
ATOM	1865	O	THR	249	6.178	9.145	32.736	1.00	41.92	B
ATOM	1866	N	ILE	250	5.857	6.979	32.214	1.00	43.64	B
ATOM	1867	CA	ILE	250	5.343	7.253	30.875	1.00	43.57	B
ATOM	1868	CB	ILE	250	5.340	5.970	30.004	1.00	43.38	B
ATOM	1869	CG2	ILE	250	4.228	5.029	30.465	1.00	41.86	B
ATOM	1870	CG1	ILE	250	5.173	6.343	28.510	1.00	41.89	B
ATOM	1871	CD1	ILE	250	5.286	5.169	27.560	1.00	39.31	B
ATOM	1872	C	ILE	250	3.922	7.805	30.983	1.00	44.06	B
ATOM	1873	O	ILE	250	3.320	8.197	29.984	1.00	43.16	B
ATOM	1874	N	ASP	251	3.402	7.834	32.209	1.00	45.37	B
ATOM	1875	CA	ASP	251	2.059	8.353	32.493	1.00	47.36	B
ATOM	1876	CB	ASP	251	1.319	7.437	33.502	1.00	47.52	B
ATOM	1877	CG	ASP	251	0.719	6.208	32.852	1.00	46.95	B
ATOM	1878	OD1	ASP	251	0.222	5.335	33.595	1.00	46.42	B
ATOM	1879	OD2	ASP	251	0.735	6.121	31.606	1.00	46.77	B
ATOM	1880	C	ASP	251	2.097	9.778	33.061	1.00	48.00	B
ATOM	1881	O	ASP	251	1.052	10.349	33.377	1.00	49.62	B
ATOM	1882	N	GLY	252	3.297	10.339	33.195	1.00	48.57	B
ATOM	1883	CA	GLY	252	3.445	11.684	33.725	1.00	48.41	B
ATOM	1884	C	GLY	252	3.519	11.749	35.243	1.00	49.25	B
ATOM	1885	O	GLY	252	3.592	12.839	35.823	1.00	48.30	B
ATOM	1886	N	GLU	253	3.489	10.584	35.890	1.00	49.52	B
ATOM	1887	CA	GLU	253	3.555	10.504	37.349	1.00	49.94	B
ATOM	1888	CB	GLU	253	2.989	9.156	37.839	1.00	51.87	B
ATOM	1889	CG	GLU	253	3.083	8.942	39.349	1.00	55.20	B
ATOM	1890	CD	GLU	253	2.805	7.498	39.764	1.00	57.60	B
ATOM	1891	OE1	GLU	253	2.837	7.204	40.981	1.00	58.27	B
ATOM	1892	OE2	GLU	253	2.558	6.655	38.875	1.00	58.42	B
ATOM	1893	C	GLU	253	4.996	10.659	37.835	1.00	49.08	B
ATOM	1894	O	GLU	253	5.948	10.301	37.136	1.00	47.88	B
ATOM	1895	N	GLU	254	5.148	11.187	39.043	1.00	48.18	B
ATOM	1896	CA	GLU	254	6.471	11.394	39.610	1.00	48.03	B
ATOM	1897	CB	GLU	254	6.633	12.854	40.000	1.00	48.74	B
ATOM	1898	CG	GLU	254	6.950	13.761	38.827	1.00	51.39	B
ATOM	1899	CD	GLU	254	6.866	15.232	39.193	1.00	53.81	B
ATOM	1900	OE1	GLU	254	7.184	15.575	40.356	1.00	54.50	B
ATOM	1901	OE2	GLU	254	6.493	16.043	38.313	1.00	54.20	B
ATOM	1902	C	GLU	254	6.817	10.497	40.797	1.00	46.73	B
ATOM	1903	O	GLU	254	6.111	10.466	41.805	1.00	46.07	B
ATOM	1904	N	LEU	255	7.918	9.763	40.651	1.00	45.44	B
ATOM	1905	CA	LEU	255	8.416	8.869	41.689	1.00	43.34	B
ATOM	1906	CB	LEU	255	8.880	7.522	41.069	1.00	42.70	B
ATOM	1907	CG	LEU	255	7.888	6.755	40.138	1.00	42.10	B
ATOM	1908	CD1	LEU	255	8.584	5.548	39.528	1.00	41.93	B
ATOM	1909	CD2	LEU	255	6.658	6.322	40.919	1.00	42.42	B
ATOM	1910	C	LEU	255	9.603	9.591	42.329	1.00	42.63	B
ATOM	1911	O	LEU	255	10.599	9.886	41.662	1.00	40.70	B

ATOM	1912	N	VAL	256	9.484	9.890	43.617	1.00	41.65	B
ATOM	1913	CA	VAL	256	10.540	10.594	44.326	1.00	41.53	B
ATOM	1914	CB	VAL	256	9.994	11.865	45.040	1.00	42.73	B
ATOM	1915	CG1	VAL	256	9.445	12.851	44.013	1.00	41.79	B
ATOM	1916	CG2	VAL	256	8.899	11.487	46.028	1.00	43.14	B
ATOM	1917	C	VAL	256	11.192	9.691	45.357	1.00	40.91	B
ATOM	1918	O	VAL	256	10.516	9.123	46.216	1.00	42.52	B
ATOM	1919	N	LYS	257	12.507	9.542	45.255	1.00	38.10	B
ATOM	1920	CA	LYS	257	13.237	8.718	46.200	1.00	35.97	B
ATOM	1921	CB	LYS	257	13.712	7.370	45.525	1.00	37.07	B
ATOM	1922	CG	LYS	257	14.482	7.490	44.219	1.00	35.97	B
ATOM	1923	CD	LYS	257	14.612	6.108	43.592	1.00	34.96	B
ATOM	1924	CE	LYS	257	15.566	6.085	42.412	1.00	36.06	B
ATOM	1925	NZ	LYS	257	15.142	6.972	41.303	1.00	38.19	B
ATOM	1926	C	LYS	257	14.408	9.497	46.777	1.00	34.33	B
ATOM	1927	O	LYS	257	15.100	10.227	46.074	1.00	35.94	B
ATOM	1928	N	ILE	258	14.618	9.345	48.074	1.00	31.24	B
ATOM	1929	CA	ILE	258	15.677	10.066	48.747	1.00	27.10	B
ATOM	1930	CB	ILE	258	15.077	10.988	49.842	1.00	28.34	B
ATOM	1931	CG2	ILE	258	16.181	11.791	50.516	1.00	26.47	B
ATOM	1932	CG1	ILE	258	14.021	11.949	49.203	1.00	27.71	B
ATOM	1933	CD1	ILE	258	13.168	12.703	50.214	1.00	25.91	B
ATOM	1934	C	ILE	258	16.695	9.136	49.382	1.00	24.38	B
ATOM	1935	O	ILE	258	16.386	8.400	50.314	1.00	22.26	B
ATOM	1936	N	GLY	259	17.917	9.182	48.872	1.00	22.97	B
ATOM	1937	CA	GLY	259	18.975	8.359	49.422	1.00	22.93	B
ATOM	1938	C	GLY	259	20.055	9.163	50.135	1.00	22.70	B
ATOM	1939	O	GLY	259	20.561	10.161	49.609	1.00	21.85	B
ATOM	1940	N	LYS	260	20.410	8.731	51.339	1.00	21.39	B
ATOM	1941	CA	LYS	260	21.441	9.412	52.112	1.00	21.77	B
ATOM	1942	CB	LYS	260	20.834	10.042	53.411	1.00	20.00	B
ATOM	1943	CG	LYS	260	21.805	10.848	54.262	1.00	17.18	B
ATOM	1944	CD	LYS	260	21.119	11.342	55.534	1.00	16.09	B
ATOM	1945	CE	LYS	260	22.049	12.181	56.417	1.00	16.97	B
ATOM	1946	NZ	LYS	260	21.341	12.724	57.641	1.00	15.85	B
ATOM	1947	C	LYS	260	22.545	8.419	52.469	1.00	21.92	B
ATOM	1948	O	LYS	260	22.284	7.303	52.938	1.00	22.32	B
ATOM	1949	N	LEU	261	23.780	8.837	52.236	1.00	19.52	B
ATOM	1950	CA	LEU	261	24.932	8.009	52.520	1.00	17.05	B
ATOM	1951	CB	LEU	261	25.693	7.741	51.235	1.00	14.85	B
ATOM	1952	CG	LEU	261	27.111	7.236	51.385	1.00	14.96	B
ATOM	1953	CD1	LEU	261	27.114	5.939	52.165	1.00	12.47	B
ATOM	1954	CD2	LEU	261	27.730	7.054	50.019	1.00	12.11	B
ATOM	1955	C	LEU	261	25.828	8.720	53.519	1.00	17.96	B
ATOM	1956	O	LEU	261	26.258	9.850	53.284	1.00	16.25	B
ATOM	1957	N	ASN	262	26.099	8.063	54.643	1.00	18.12	B
ATOM	1958	CA	ASN	262	26.970	8.640	55.670	1.00	18.04	B
ATOM	1959	CB	ASN	262	26.336	8.512	57.080	1.00	15.45	B
ATOM	1960	CG	ASN	262	24.943	9.103	57.152	1.00	17.34	B
ATOM	1961	OD1	ASN	262	23.957	8.381	57.282	1.00	17.52	B
ATOM	1962	ND2	ASN	262	24.855	10.420	57.070	1.00	17.02	B
ATOM	1963	C	ASN	262	28.327	7.929	55.664	1.00	18.26	B
ATOM	1964	O	ASN	262	28.399	6.697	55.735	1.00	16.87	B
ATOM	1965	N	LEU	263	29.394	8.717	55.564	1.00	18.04	B
ATOM	1966	CA	LEU	263	30.759	8.200	55.560	1.00	17.90	B
ATOM	1967	CB	LEU	263	31.482	8.723	54.339	1.00	15.70	B
ATOM	1968	CG	LEU	263	30.717	8.283	53.075	1.00	17.05	B
ATOM	1969	CD1	LEU	263	31.255	8.961	51.853	1.00	16.38	B
ATOM	1970	CD2	LEU	263	30.812	6.754	52.929	1.00	18.46	B
ATOM	1971	C	LEU	263	31.411	8.688	56.849	1.00	18.79	B
ATOM	1972	O	LEU	263	31.712	9.873	56.992	1.00	20.38	B
ATOM	1973	N	VAL	264	31.614	7.774	57.794	1.00	18.49	B
ATOM	1974	CA	VAL	264	32.183	8.128	59.093	1.00	18.30	B
ATOM	1975	CB	VAL	264	31.335	7.529	60.228	1.00	18.68	B
ATOM	1976	CG1	VAL	264	31.752	8.115	61.561	1.00	17.56	B
ATOM	1977	CG2	VAL	264	29.858	7.772	59.955	1.00	21.14	B
ATOM	1978	C	VAL	264	33.627	7.696	59.333	1.00	19.31	B
ATOM	1979	O	VAL	264	33.952	6.513	59.210	1.00	19.80	B
ATOM	1980	N	ASP	265	34.478	8.667	59.680	1.00	17.61	B
ATOM	1981	CA	ASP	265	35.880	8.419	59.995	1.00	15.36	B
ATOM	1982	CB	ASP	265	36.771	9.484	59.355	1.00	14.42	B
ATOM	1983	CG	ASP	265	38.258	9.279	59.658	1.00	16.29	B
ATOM	1984	OD1	ASP	265	38.583	8.741	60.736	1.00	19.48	B

ATOM	1985	OD2	ASP	265	39.110	9.677	58.832	1.00	16.17	B
ATOM	1986	C	ASP	265	35.971	8.507	61.528	1.00	15.62	B
ATOM	1987	O	ASP	265	36.119	9.593	62.086	1.00	17.19	B
ATOM	1988	N	LEU	266	35.891	7.367	62.205	1.00	13.53	B
ATOM	1989	CA	LEU	266	35.930	7.357	63.666	1.00	12.99	B
ATOM	1990	CB	LEU	266	35.555	5.913	64.239	1.00	9.90	B
ATOM	1991	CG	LEU	266	34.172	5.339	63.898	1.00	12.88	B
ATOM	1992	CD1	LEU	266	34.070	3.881	64.374	1.00	12.44	B
ATOM	1993	CD2	LEU	266	33.088	6.185	64.542	1.00	11.19	B
ATOM	1994	C	LEU	266	37.277	7.783	64.240	1.00	11.25	B
ATOM	1995	O	LEU	266	38.274	7.867	63.532	1.00	7.77	B
ATOM	1996	N	ALA	267	37.263	8.059	65.539	1.00	10.58	B
ATOM	1997	CA	ALA	267	38.453	8.422	66.284	1.00	13.04	B
ATOM	1998	CB	ALA	267	38.057	9.029	67.634	1.00	11.27	B
ATOM	1999	C	ALA	267	39.221	7.125	66.507	1.00	14.13	B
ATOM	2000	O	ALA	267	38.610	6.077	66.718	1.00	16.34	B
ATOM	2001	N	GLY	268	40.546	7.190	66.475	1.00	14.85	B
ATOM	2002	CA	GLY	268	41.347	5.999	66.688	1.00	17.83	B
ATOM	2003	C	GLY	268	40.934	5.198	67.909	1.00	20.15	B
ATOM	2004	O	GLY	268	40.663	5.760	68.978	1.00	21.52	B
ATOM	2005	N	SER	269	40.918	3.878	67.773	1.00	20.60	B
ATOM	2006	CA	SER	269	40.500	3.017	68.878	1.00	23.05	B
ATOM	2007	CB	SER	269	39.929	1.721	68.324	1.00	20.23	B
ATOM	2008	OG	SER	269	40.842	1.099	67.442	1.00	17.43	B
ATOM	2009	C	SER	269	41.546	2.678	69.941	1.00	26.49	B
ATOM	2010	O	SER	269	41.227	1.969	70.903	1.00	27.04	B
ATOM	2011	N	GLU	270	42.775	3.171	69.781	1.00	29.47	B
ATOM	2012	CA	GLU	270	43.848	2.887	70.743	1.00	32.95	B
ATOM	2013	CB	GLU	270	45.234	3.432	70.210	1.00	32.65	B
ATOM	2014	CG	GLU	270	45.405	4.968	70.193	1.00	30.27	B
ATOM	2015	CD	GLU	270	44.822	5.656	68.963	1.00	30.89	B
ATOM	2016	OE1	GLU	270	44.879	6.908	68.911	1.00	32.19	B
ATOM	2017	OE2	GLU	270	44.315	4.961	68.052	1.00	28.80	B
ATOM	2018	C	GLU	270	43.560	3.472	72.129	1.00	36.87	B
ATOM	2019	O	GLU	270	43.380	4.681	72.277	1.00	39.21	B
ATOM	2020	N	ASN	271	43.503	2.613	73.143	1.00	40.27	B
ATOM	2021	CA	ASN	271	43.238	3.062	74.515	1.00	42.68	B
ATOM	2022	CB	ASN	271	42.196	2.131	75.222	1.00	43.15	B
ATOM	2023	CG	ASN	271	40.798	2.244	74.621	1.00	45.39	B
ATOM	2024	OD1	ASN	271	40.230	3.337	74.540	1.00	46.39	B
ATOM	2025	ND2	ASN	271	40.232	1.109	74.210	1.00	43.39	B
ATOM	2026	C	ASN	271	44.528	3.093	75.331	1.00	43.55	B
ATOM	2027	O	ASN	271	45.603	2.746	74.833	1.00	43.93	B
ATOM	2028	N	ASN	287	41.588	11.864	79.666	1.00	44.94	B
ATOM	2029	CA	ASN	287	40.716	12.252	78.558	1.00	45.22	B
ATOM	2030	CB	ASN	287	41.514	13.086	77.476	1.00	48.29	B
ATOM	2031	CG	ASN	287	42.261	14.276	78.074	1.00	50.68	B
ATOM	2032	OD1	ASN	287	43.249	14.106	78.796	1.00	51.76	B
ATOM	2033	ND2	ASN	287	41.791	15.488	77.774	1.00	51.75	B
ATOM	2034	C	ASN	287	40.091	11.016	77.897	1.00	42.90	B
ATOM	2035	O	ASN	287	40.787	10.182	77.315	1.00	42.06	B
ATOM	2036	N	ILE	288	38.771	10.914	77.995	1.00	40.12	B
ATOM	2037	CA	ILE	288	38.034	9.794	77.424	1.00	36.62	B
ATOM	2038	CB	ILE	288	37.110	9.146	78.479	1.00	37.65	B
ATOM	2039	CG2	ILE	288	37.911	8.154	79.325	1.00	38.70	B
ATOM	2040	CG1	ILE	288	36.464	10.252	79.390	1.00	36.64	B
ATOM	2041	CD1	ILE	288	35.583	11.252	78.657	1.00	36.28	B
ATOM	2042	C	ILE	288	37.183	10.200	76.230	1.00	33.35	B
ATOM	2043	O	ILE	288	36.763	11.356	76.100	1.00	34.53	B
ATOM	2044	N	ASN	289	36.938	9.252	75.342	1.00	27.16	B
ATOM	2045	CA	ASN	289	36.112	9.564	74.199	1.00	23.25	B
ATOM	2046	CB	ASN	289	36.731	9.052	72.954	1.00	20.82	B
ATOM	2047	CG	ASN	289	36.172	9.721	71.712	1.00	19.85	B
ATOM	2048	OD1	ASN	289	36.929	10.208	70.878	1.00	19.66	B
ATOM	2049	ND2	ASN	289	34.846	9.737	71.576	1.00	17.37	B
ATOM	2050	C	ASN	289	34.763	8.912	74.459	1.00	20.79	B
ATOM	2051	O	ASN	289	34.553	7.735	74.170	1.00	18.65	B
ATOM	2052	N	GLN	290	33.863	9.694	75.042	1.00	19.57	B
ATOM	2053	CA	GLN	290	32.537	9.216	75.379	1.00	19.29	B
ATOM	2054	CB	GLN	290	31.678	10.366	75.901	1.00	19.26	B
ATOM	2055	CG	GLN	290	30.278	9.942	76.312	1.00	19.65	B
ATOM	2056	CD	GLN	290	30.265	8.891	77.423	1.00	20.79	B
ATOM	2057	OE1	GLN	290	29.211	8.339	77.754	1.00	21.88	B

ATOM	2058	NE2	GLN	290	31.427	8.621	78.006	1.00	18.18	B
ATOM	2059	C	GLN	290	31.830	8.538	74.214	1.00	18.80	B
ATOM	2060	O	GLN	290	31.199	7.502	74.397	1.00	17.47	B
ATOM	2061	N	SER	291	31.939	9.122	73.021	1.00	18.97	B
ATOM	2062	CA	SER	291	31.289	8.565	71.841	1.00	18.84	B
ATOM	2063	CB	SER	291	31.326	9.565	70.646	1.00	19.15	B
ATOM	2064	OG	SER	291	30.347	10.593	70.784	1.00	19.00	B
ATOM	2065	C	SER	291	31.897	7.239	71.420	1.00	19.68	B
ATOM	2066	O	SER	291	31.173	6.323	71.027	1.00	21.26	B
ATOM	2067	N	LEU	292	33.219	7.131	71.494	1.00	18.43	B
ATOM	2068	CA	LEU	292	33.872	5.888	71.128	1.00	17.73	B
ATOM	2069	CB	LEU	292	35.361	6.070	71.140	1.00	15.77	B
ATOM	2070	CG	LEU	292	36.119	4.969	70.418	1.00	15.31	B
ATOM	2071	CD1	LEU	292	35.703	4.951	68.953	1.00	11.07	B
ATOM	2072	CD2	LEU	292	37.621	5.213	70.548	1.00	16.30	B
ATOM	2073	C	LEU	292	33.461	4.827	72.159	1.00	19.37	B
ATOM	2074	O	LEU	292	33.107	3.698	71.814	1.00	20.03	B
ATOM	2075	N	LEU	293	33.504	5.219	73.430	1.00	19.01	B
ATOM	2076	CA	LEU	293	33.137	4.357	74.531	1.00	18.18	B
ATOM	2077	CB	LEU	293	33.194	5.140	75.819	1.00	16.50	B
ATOM	2078	CG	LEU	293	34.193	4.752	76.903	1.00	18.80	B
ATOM	2079	CD1	LEU	293	35.291	3.824	76.354	1.00	14.59	B
ATOM	2080	CD2	LEU	293	34.789	6.039	77.485	1.00	18.33	B
ATOM	2081	C	LEU	293	31.724	3.828	74.326	1.00	20.79	B
ATOM	2082	O	LEU	293	31.446	2.629	74.480	1.00	21.79	B
ATOM	2083	N	THR	294	30.824	4.730	73.972	1.00	20.82	B
ATOM	2084	CA	THR	294	29.444	4.348	73.785	1.00	21.70	B
ATOM	2085	CB	THR	294	28.556	5.607	73.770	1.00	21.45	B
ATOM	2086	OG1	THR	294	28.737	6.305	75.012	1.00	20.05	B
ATOM	2087	CG2	THR	294	27.085	5.243	73.638	1.00	23.08	B
ATOM	2088	C	THR	294	29.245	3.488	72.541	1.00	22.57	B
ATOM	2089	O	THR	294	28.410	2.589	72.541	1.00	24.83	B
ATOM	2090	N	LEU	295	30.028	3.726	71.492	1.00	22.48	B
ATOM	2091	CA	LEU	295	29.888	2.929	70.278	1.00	20.67	B
ATOM	2092	CB	LEU	295	30.896	3.354	69.239	1.00	16.50	B
ATOM	2093	CG	LEU	295	30.872	2.542	67.933	1.00	15.31	B
ATOM	2094	CD1	LEU	295	29.480	2.540	67.301	1.00	9.83	B
ATOM	2095	CD2	LEU	295	31.901	3.126	66.996	1.00	13.69	B
ATOM	2096	C	LEU	295	30.072	1.453	70.614	1.00	21.75	B
ATOM	2097	O	LEU	295	29.261	0.620	70.222	1.00	22.82	B
ATOM	2098	N	GLY	296	31.141	1.141	71.345	1.00	22.87	B
ATOM	2099	CA	GLY	296	31.402	-0.230	71.753	1.00	21.35	B
ATOM	2100	C	GLY	296	30.318	-0.785	72.668	1.00	20.58	B
ATOM	2101	O	GLY	296	29.960	-1.950	72.566	1.00	22.84	B
ATOM	2102	N	ARG	297	29.782	0.034	73.562	1.00	19.00	B
ATOM	2103	CA	ARG	297	28.735	-0.441	74.462	1.00	18.91	B
ATOM	2104	CB	ARG	297	28.530	0.539	75.601	1.00	17.91	B
ATOM	2105	CG	ARG	297	29.645	0.523	76.596	1.00	17.55	B
ATOM	2106	CD	ARG	297	29.622	1.775	77.433	1.00	21.12	B
ATOM	2107	NE	ARG	297	30.783	1.860	78.311	1.00	20.84	B
ATOM	2108	CZ	ARG	297	31.212	2.987	78.862	1.00	19.95	B
ATOM	2109	NH1	ARG	297	30.567	4.118	78.614	1.00	19.89	B
ATOM	2110	NH2	ARG	297	32.274	2.982	79.661	1.00	15.55	B
ATOM	2111	C	ARG	297	27.419	-0.662	73.733	1.00	18.05	B
ATOM	2112	O	ARG	297	26.581	-1.440	74.177	1.00	18.18	B
ATOM	2113	N	VAL	298	27.235	0.035	72.618	1.00	19.06	B
ATOM	2114	CA	VAL	298	26.019	-0.106	71.823	1.00	17.97	B
ATOM	2115	CB	VAL	298	25.816	1.111	70.885	1.00	15.95	B
ATOM	2116	CG1	VAL	298	24.691	0.843	69.899	1.00	13.08	B
ATOM	2117	CG2	VAL	298	25.507	2.350	71.710	1.00	14.44	B
ATOM	2118	C	VAL	298	26.140	-1.377	70.985	1.00	19.67	B
ATOM	2119	O	VAL	298	25.153	-2.075	70.749	1.00	21.91	B
ATOM	2120	N	ILE	299	27.356	-1.686	70.544	1.00	19.47	B
ATOM	2121	CA	ILE	299	27.570	-2.879	69.736	1.00	21.25	B
ATOM	2122	CB	ILE	299	28.973	-2.830	69.068	1.00	21.35	B
ATOM	2123	CG2	ILE	299	29.354	-4.192	68.502	1.00	19.14	B
ATOM	2124	CG1	ILE	299	28.950	-1.752	67.932	1.00	19.67	B
ATOM	2125	CD1	ILE	299	30.316	-1.238	67.523	1.00	19.64	B
ATOM	2126	C	ILE	299	27.399	-4.122	70.610	1.00	22.50	B
ATOM	2127	O	ILE	299	26.774	-5.102	70.206	1.00	21.52	B
ATOM	2128	N	THR	300	27.936	-4.057	71.821	1.00	23.04	B
ATOM	2129	CA	THR	300	27.827	-5.153	72.763	1.00	23.72	B
ATOM	2130	CB	THR	300	28.521	-4.787	74.068	1.00	23.18	B

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ATOM   2131  OG1 THR   300      29.923  -4.646  73.811  1.00 21.92      B
ATOM   2132  CG2 THR   300      28.284  -5.841  75.138  1.00 17.93      B
ATOM   2133  C   THR   300      26.353  -5.447  73.020  1.00 27.59      B
ATOM   2134  O   THR   300      25.878  -6.563  72.787  1.00 27.46      B
ATOM   2135  N   ALA   301      25.626  -4.438  73.480  1.00 29.03      B
ATOM   2136  CA  ALA   301      24.206  -4.600  73.754  1.00 30.76      B
ATOM   2137  CB  ALA   301      23.598  -3.262  74.139  1.00 31.16      B
ATOM   2138  C   ALA   301      23.437  -5.196  72.573  1.00 32.99      B
ATOM   2139  O   ALA   301      22.545  -6.017  72.772  1.00 35.01      B
ATOM   2140  N   LEU   302      23.770  -4.780  71.351  1.00 34.50      B
ATOM   2141  CA  LEU   302      23.088  -5.279  70.152  1.00 34.70      B
ATOM   2142  CB  LEU   302      23.440  -4.425  68.943  1.00 35.01      B
ATOM   2143  CG  LEU   302      22.840  -2.999  68.895  1.00 35.55      B
ATOM   2144  CD1 LEU   302      23.474  -2.227  67.759  1.00 36.40      B
ATOM   2145  CD2 LEU   302      21.334  -3.063  68.714  1.00 33.89      B
ATOM   2146  C   LEU   302      23.451  -6.721  69.855  1.00 35.87      B
ATOM   2147  O   LEU   302      22.590  -7.547  69.549  1.00 36.50      B
ATOM   2148  N   VAL   303      24.742  -7.008  69.941  1.00 36.97      B
ATOM   2149  CA  VAL   303      25.271  -8.339  69.691  1.00 36.81      B
ATOM   2150  CB  VAL   303      26.818  -8.289  69.707  1.00 36.26      B
ATOM   2151  CG1 VAL   303      27.402  -9.658  69.961  1.00 35.12      B
ATOM   2152  CG2 VAL   303      27.316  -7.726  68.384  1.00 35.06      B
ATOM   2153  C   VAL   303      24.757  -9.359  70.711  1.00 38.19      B
ATOM   2154  O   VAL   303      24.495 -10.506  70.368  1.00 39.57      B
ATOM   2155  N   GLU   304      24.597  -8.928  71.957  1.00 39.43      B
ATOM   2156  CA  GLU   304      24.129  -9.796  73.032  1.00 40.38      B
ATOM   2157  CB  GLU   304      24.768  -9.359  74.350  1.00 41.03      B
ATOM   2158  CG  GLU   304      26.290  -9.464  74.347  1.00 42.14      B
ATOM   2159  CD  GLU   304      26.889  -9.210  75.713  1.00 43.89      B
ATOM   2160  OE1 GLU   304      28.116  -9.390  75.879  1.00 42.77      B
ATOM   2161  OE2 GLU   304      26.127  -8.827  76.625  1.00 45.66      B
ATOM   2162  C   GLU   304      22.612  -9.817  73.179  1.00 41.20      B
ATOM   2163  O   GLU   304      22.071 -10.477  74.062  1.00 39.68      B
ATOM   2164  N   ARG   305      21.932  -9.088  72.305  1.00 44.11      B
ATOM   2165  CA  ARG   305      20.474  -9.004  72.310  1.00 46.91      B
ATOM   2166  CB  ARG   305      19.835 -10.408  71.997  1.00 48.72      B
ATOM   2167  CG  ARG   305      20.520 -11.222  70.897  1.00 52.86      B
ATOM   2168  CD  ARG   305      20.686 -10.461  69.579  1.00 56.32      B
ATOM   2169  NE  ARG   305      21.395 -11.268  68.582  1.00 59.70      B
ATOM   2170  CZ  ARG   305      21.970 -10.782  67.483  1.00 61.81      B
ATOM   2171  NH1 ARG   305      21.926  -9.479  67.221  1.00 61.95      B
ATOM   2172  NH2 ARG   305      22.605 -11.601  66.649  1.00 61.81      B
ATOM   2173  C   ARG   305      19.890  -8.469  73.620  1.00 47.13      B
ATOM   2174  O   ARG   305      18.784  -8.840  73.996  1.00 48.14      B
ATOM   2175  N   THR   306      20.621  -7.599  74.311  1.00 48.36      B
ATOM   2176  CA  THR   306      20.135  -7.027  75.568  1.00 49.45      B
ATOM   2177  CB  THR   306      21.275  -6.367  76.356  1.00 49.08      B
ATOM   2178  OG1 THR   306      22.429  -7.214  76.326  1.00 49.36      B
ATOM   2179  CG2 THR   306      20.862  -6.155  77.802  1.00 48.92      B
ATOM   2180  C   THR   306      19.066  -5.972  75.262  1.00 50.64      B
ATOM   2181  O   THR   306      19.275  -5.091  74.428  1.00 51.81      B
ATOM   2182  N   PRO   307      17.910  -6.044  75.942  1.00 51.76      B
ATOM   2183  CD  PRO   307      17.651  -6.959  77.068  1.00 52.91      B
ATOM   2184  CA  PRO   307      16.779  -5.119  75.761  1.00 52.01      B
ATOM   2185  CB  PRO   307      15.945  -5.358  76.995  1.00 52.53      B
ATOM   2186  CG  PRO   307      16.158  -6.818  77.257  1.00 53.28      B
ATOM   2187  C   PRO   307      17.124  -3.638  75.585  1.00 51.42      B
ATOM   2188  O   PRO   307      16.624  -2.983  74.664  1.00 51.33      B
ATOM   2189  N   HIS   308      17.973  -3.115  76.466  1.00 49.88      B
ATOM   2190  CA  HIS   308      18.359  -1.711  76.410  1.00 47.29      B
ATOM   2191  CB  HIS   308      18.432  -1.141  77.832  1.00 50.27      B
ATOM   2192  CG  HIS   308      18.812   0.306  77.877  1.00 54.50      B
ATOM   2193  CD2 HIS   308      19.992   0.909  78.158  1.00 55.48      B
ATOM   2194  ND1 HIS   308      17.931   1.318  77.559  1.00 55.94      B
ATOM   2195  CE1 HIS   308      18.552   2.482  77.641  1.00 56.20      B
ATOM   2196  NE2 HIS   308      19.804   2.262  78.003  1.00 56.35      B
ATOM   2197  C   HIS   308      19.685  -1.445  75.690  1.00 43.71      B
ATOM   2198  O   HIS   308      20.709  -2.061  75.991  1.00 43.17      B
ATOM   2199  N   VAL   309      19.649  -0.517  74.737  1.00 39.63      B
ATOM   2200  CA  VAL   309      20.829  -0.117  73.964  1.00 34.96      B
ATOM   2201  CB  VAL   309      20.561  -0.206  72.449  1.00 34.96      B
ATOM   2202  CG1 VAL   309      21.858   0.013  71.675  1.00 34.27      B
ATOM   2203  CG2 VAL   309      19.934  -1.548  72.114  1.00 32.68      B
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ATOM	2204	C	VAL	309	21.086	1.344	74.336	1.00	31.77	B
ATOM	2205	O	VAL	309	20.237	2.204	74.102	1.00	30.77	B
ATOM	2206	N	PRO	310	22.266	1.642	74.906	1.00	29.55	B
ATOM	2207	CD	PRO	310	23.347	0.670	75.171	1.00	27.65	B
ATOM	2208	CA	PRO	310	22.652	2.997	75.335	1.00	29.03	B
ATOM	2209	CB	PRO	310	23.856	2.732	76.230	1.00	29.20	B
ATOM	2210	CG	PRO	310	24.518	1.555	75.539	1.00	27.40	B
ATOM	2211	C	PRO	310	22.949	4.064	74.268	1.00	28.13	B
ATOM	2212	O	PRO	310	23.960	4.760	74.357	1.00	27.93	B
ATOM	2213	N	TYR	311	22.064	4.198	73.284	1.00	27.73	B
ATOM	2214	CA	TYR	311	22.217	5.175	72.203	1.00	28.46	B
ATOM	2215	CB	TYR	311	20.949	5.195	71.291	1.00	29.00	B
ATOM	2216	CG	TYR	311	20.724	3.960	70.450	1.00	32.30	B
ATOM	2217	CD1	TYR	311	21.600	3.631	69.413	1.00	32.05	B
ATOM	2218	CE1	TYR	311	21.393	2.492	68.628	1.00	34.37	B
ATOM	2219	CD2	TYR	311	19.627	3.119	70.686	1.00	31.31	B
ATOM	2220	CE2	TYR	311	19.411	1.979	69.908	1.00	32.07	B
ATOM	2221	CZ	TYR	311	20.299	1.669	68.882	1.00	34.42	B
ATOM	2222	OH	TYR	311	20.120	0.531	68.122	1.00	35.43	B
ATOM	2223	C	TYR	311	22.458	6.611	72.678	1.00	28.67	B
ATOM	2224	O	TYR	311	23.343	7.296	72.177	1.00	27.07	B
ATOM	2225	N	ARG	312	21.652	7.059	73.635	1.00	29.15	B
ATOM	2226	CA	ARG	312	21.716	8.425	74.143	1.00	29.95	B
ATOM	2227	CB	ARG	312	20.481	8.724	74.961	1.00	32.31	B
ATOM	2228	CG	ARG	312	19.189	8.626	74.196	1.00	36.65	B
ATOM	2229	CD	ARG	312	18.046	8.529	75.169	1.00	40.81	B
ATOM	2230	NE	ARG	312	16.862	7.919	74.577	1.00	43.18	B
ATOM	2231	CZ	ARG	312	15.951	7.251	75.278	1.00	45.73	B
ATOM	2232	NH1	ARG	312	16.100	7.108	76.597	1.00	44.15	B
ATOM	2233	NH2	ARG	312	14.888	6.737	74.664	1.00	45.91	B
ATOM	2234	C	ARG	312	22.926	8.811	74.969	1.00	28.83	B
ATOM	2235	O	ARG	312	23.104	9.991	75.276	1.00	29.69	B
ATOM	2236	N	GLU	313	23.755	7.843	75.340	1.00	26.62	B
ATOM	2237	CA	GLU	313	24.917	8.160	76.153	1.00	22.31	B
ATOM	2238	CB	GLU	313	25.419	6.929	76.814	1.00	22.37	B
ATOM	2239	CG	GLU	313	24.550	6.521	77.994	1.00	24.92	B
ATOM	2240	CD	GLU	313	24.871	5.136	78.554	1.00	26.13	B
ATOM	2241	OE1	GLU	313	26.060	4.823	78.755	1.00	27.91	B
ATOM	2242	OE2	GLU	313	23.926	4.365	78.813	1.00	27.77	B
ATOM	2243	C	GLU	313	26.031	8.873	75.403	1.00	21.16	B
ATOM	2244	O	GLU	313	27.096	9.122	75.963	1.00	21.76	B
ATOM	2245	N	SER	314	25.789	9.222	74.144	1.00	18.52	B
ATOM	2246	CA	SER	314	26.796	9.935	73.375	1.00	19.81	B
ATOM	2247	CB	SER	314	27.966	8.992	72.968	1.00	20.10	B
ATOM	2248	OG	SER	314	27.731	8.382	71.710	1.00	19.29	B
ATOM	2249	C	SER	314	26.206	10.583	72.130	1.00	20.60	B
ATOM	2250	O	SER	314	25.198	10.126	71.597	1.00	19.90	B
ATOM	2251	N	LYS	315	26.854	11.654	71.676	1.00	20.92	B
ATOM	2252	CA	LYS	315	26.412	12.395	70.504	1.00	20.48	B
ATOM	2253	CB	LYS	315	27.264	13.689	70.329	1.00	20.26	B
ATOM	2254	CG	LYS	315	27.318	14.572	71.556	1.00	19.73	B
ATOM	2255	CD	LYS	315	25.936	14.893	72.074	1.00	22.19	B
ATOM	2256	CE	LYS	315	25.984	15.989	73.129	1.00	23.41	B
ATOM	2257	NZ	LYS	315	26.408	17.293	72.528	1.00	26.09	B
ATOM	2258	C	LYS	315	26.513	11.560	69.239	1.00	19.78	B
ATOM	2259	O	LYS	315	25.626	11.614	68.373	1.00	20.29	B
ATOM	2260	N	LEU	316	27.598	10.796	69.130	1.00	17.65	B
ATOM	2261	CA	LEU	316	27.808	9.962	67.955	1.00	17.80	B
ATOM	2262	CB	LEU	316	29.209	9.245	68.013	1.00	16.46	B
ATOM	2263	CG	LEU	316	29.602	8.339	66.775	1.00	15.01	B
ATOM	2264	CD1	LEU	316	29.683	9.151	65.507	1.00	14.12	B
ATOM	2265	CD2	LEU	316	30.937	7.695	67.030	1.00	17.53	B
ATOM	2266	C	LEU	316	26.698	8.926	67.798	1.00	17.14	B
ATOM	2267	O	LEU	316	26.060	8.854	66.742	1.00	17.17	B
ATOM	2268	N	THR	317	26.462	8.137	68.844	1.00	17.69	B
ATOM	2269	CA	THR	317	25.439	7.106	68.777	1.00	19.04	B
ATOM	2270	CB	THR	317	25.525	6.124	69.966	1.00	21.44	B
ATOM	2271	OG1	THR	317	25.617	6.848	71.198	1.00	21.96	B
ATOM	2272	CG2	THR	317	26.743	5.206	69.804	1.00	21.41	B
ATOM	2273	C	THR	317	24.031	7.659	68.659	1.00	18.09	B
ATOM	2274	O	THR	317	23.155	6.990	68.130	1.00	17.17	B
ATOM	2275	N	ARG	318	23.800	8.877	69.134	1.00	19.16	B
ATOM	2276	CA	ARG	318	22.469	9.460	68.986	1.00	20.49	B

ATOM	2277	CB	ARG	318	22.283	10.654	69.927	1.00	22.85	B
ATOM	2278	CG	ARG	318	22.155	10.218	71.387	1.00	28.27	B
ATOM	2279	CD	ARG	318	21.942	11.375	72.318	1.00	31.62	B
ATOM	2280	NE	ARG	318	20.929	12.277	71.788	1.00	39.60	B
ATOM	2281	CZ	ARG	318	20.361	13.261	72.479	1.00	40.99	B
ATOM	2282	NH1	ARG	318	20.703	13.474	73.746	1.00	41.19	B
ATOM	2283	NH2	ARG	318	19.454	14.034	71.894	1.00	41.05	B
ATOM	2284	C	ARG	318	22.288	9.873	67.525	1.00	20.16	B
ATOM	2285	O	ARG	318	21.237	9.648	66.929	1.00	21.26	B
ATOM	2286	N	ILE	319	23.332	10.435	66.932	1.00	18.27	B
ATOM	2287	CA	ILE	319	23.255	10.843	65.539	1.00	18.18	B
ATOM	2288	CB	ILE	319	24.505	11.665	65.132	1.00	17.80	B
ATOM	2289	CG2	ILE	319	24.482	11.913	63.619	1.00	17.11	B
ATOM	2290	CG1	ILE	319	24.561	13.006	65.928	1.00	17.07	B
ATOM	2291	CD1	ILE	319	25.901	13.727	65.838	1.00	14.30	B
ATOM	2292	C	ILE	319	23.134	9.663	64.550	1.00	18.77	B
ATOM	2293	O	ILE	319	22.397	9.753	63.569	1.00	16.28	B
ATOM	2294	N	LEU	320	23.860	8.571	64.808	1.00	18.72	B
ATOM	2295	CA	LEU	320	23.874	7.415	63.905	1.00	18.52	B
ATOM	2296	CB	LEU	320	25.323	7.003	63.621	1.00	14.27	B
ATOM	2297	CG	LEU	320	26.321	8.000	63.025	1.00	16.38	B
ATOM	2298	CD1	LEU	320	27.707	7.354	63.017	1.00	13.61	B
ATOM	2299	CD2	LEU	320	25.905	8.426	61.605	1.00	14.32	B
ATOM	2300	C	LEU	320	23.113	6.159	64.354	1.00	21.16	B
ATOM	2301	O	LEU	320	23.308	5.087	63.780	1.00	21.77	B
ATOM	2302	N	GLN	321	22.249	6.277	65.357	1.00	22.79	B
ATOM	2303	CA	GLN	321	21.519	5.114	65.848	1.00	25.68	B
ATOM	2304	CB	GLN	321	20.531	5.524	66.954	1.00	28.52	B
ATOM	2305	CG	GLN	321	19.448	6.490	66.535	1.00	32.15	B
ATOM	2306	CD	GLN	321	18.539	6.843	67.700	1.00	35.99	B
ATOM	2307	OE1	GLN	321	17.953	5.954	68.332	1.00	33.89	B
ATOM	2308	NE2	GLN	321	18.417	8.144	67.997	1.00	36.73	B
ATOM	2309	C	GLN	321	20.790	4.254	64.813	1.00	25.53	B
ATOM	2310	O	GLN	321	20.625	3.056	65.029	1.00	25.73	B
ATOM	2311	N	ASP	322	20.353	4.837	63.701	1.00	26.46	B
ATOM	2312	CA	ASP	322	19.659	4.040	62.695	1.00	28.33	B
ATOM	2313	CB	ASP	322	18.913	4.934	61.681	1.00	29.02	B
ATOM	2314	CG	ASP	322	17.894	4.152	60.847	1.00	30.51	B
ATOM	2315	OD1	ASP	322	17.880	4.308	59.604	1.00	31.51	B
ATOM	2316	OD2	ASP	322	17.100	3.384	61.434	1.00	29.46	B
ATOM	2317	C	ASP	322	20.661	3.152	61.959	1.00	29.44	B
ATOM	2318	O	ASP	322	20.284	2.195	61.280	1.00	29.55	B
ATOM	2319	N	SER	323	21.943	3.480	62.095	1.00	29.59	B
ATOM	2320	CA	SER	323	22.999	2.705	61.458	1.00	28.78	B
ATOM	2321	CB	SER	323	24.172	3.594	61.165	1.00	27.31	B
ATOM	2322	OG	SER	323	23.845	4.545	60.178	1.00	26.34	B
ATOM	2323	C	SER	323	23.453	1.519	62.322	1.00	29.30	B
ATOM	2324	O	SER	323	24.234	0.687	61.875	1.00	28.51	B
ATOM	2325	N	LEU	324	22.967	1.445	63.558	1.00	30.19	B
ATOM	2326	CA	LEU	324	23.338	0.354	64.451	1.00	30.51	B
ATOM	2327	CB	LEU	324	24.110	0.893	65.662	1.00	30.62	B
ATOM	2328	CG	LEU	324	25.577	1.365	65.474	1.00	29.76	B
ATOM	2329	CD1	LEU	324	25.670	2.412	64.401	1.00	31.76	B
ATOM	2330	CD2	LEU	324	26.085	1.928	66.775	1.00	28.62	B
ATOM	2331	C	LEU	324	22.113	-0.419	64.927	1.00	31.44	B
ATOM	2332	O	LEU	324	21.611	-0.184	66.026	1.00	32.71	B
ATOM	2333	N	GLY	325	21.642	-1.347	64.095	1.00	31.87	B
ATOM	2334	CA	GLY	325	20.479	-2.148	64.444	1.00	30.03	B
ATOM	2335	C	GLY	325	19.190	-1.440	64.082	1.00	29.89	B
ATOM	2336	O	GLY	325	18.160	-1.636	64.727	1.00	29.38	B
ATOM	2337	N	GLY	326	19.253	-0.614	63.042	1.00	29.59	B
ATOM	2338	CA	GLY	326	18.092	0.139	62.603	1.00	27.99	B
ATOM	2339	C	GLY	326	17.706	-0.236	61.193	1.00	27.84	B
ATOM	2340	O	GLY	326	17.896	-1.378	60.811	1.00	28.56	B
ATOM	2341	N	ARG	327	17.197	0.719	60.418	1.00	26.60	B
ATOM	2342	CA	ARG	327	16.763	0.456	59.046	1.00	27.36	B
ATOM	2343	CB	ARG	327	15.451	1.234	58.745	1.00	30.55	B
ATOM	2344	CG	ARG	327	14.534	1.451	59.943	1.00	34.58	B
ATOM	2345	CD	ARG	327	13.775	0.198	60.367	1.00	40.44	B
ATOM	2346	NE	ARG	327	12.359	0.271	60.014	1.00	43.41	B
ATOM	2347	CZ	ARG	327	11.898	0.209	58.768	1.00	47.99	B
ATOM	2348	NH1	ARG	327	12.741	0.071	57.751	1.00	49.86	B
ATOM	2349	NH2	ARG	327	10.592	0.285	58.535	1.00	48.98	B

ATOM	2350	C	ARG	327	17.796	0.811	57.967	1.00	27.20	B
ATOM	2351	O	ARG	327	17.521	0.680	56.775	1.00	27.07	B
ATOM	2352	N	THR	328	18.977	1.257	58.379	1.00	26.89	B
ATOM	2353	CA	THR	328	20.028	1.646	57.441	1.00	25.49	B
ATOM	2354	CB	THR	328	20.870	2.813	58.024	1.00	27.20	B
ATOM	2355	OG1	THR	328	20.024	3.944	58.252	1.00	29.46	B
ATOM	2356	CG2	THR	328	21.992	3.210	57.072	1.00	26.15	B
ATOM	2357	C	THR	328	20.974	0.492	57.125	1.00	24.96	B
ATOM	2358	O	THR	328	21.238	-0.346	57.984	1.00	24.98	B
ATOM	2359	N	ARG	329	21.465	0.431	55.890	1.00	23.74	B
ATOM	2360	CA	ARG	329	22.426	-0.610	55.543	1.00	24.57	B
ATOM	2361	CB	ARG	329	22.551	-0.842	54.014	1.00	26.29	B
ATOM	2362	CG	ARG	329	23.421	-2.071	53.721	1.00	31.07	B
ATOM	2363	CD	ARG	329	24.277	-1.980	52.461	1.00	34.15	B
ATOM	2364	NE	ARG	329	23.590	-2.447	51.259	1.00	37.59	B
ATOM	2365	CZ	ARG	329	24.217	-2.885	50.168	1.00	38.17	B
ATOM	2366	NH1	ARG	329	25.547	-2.923	50.124	1.00	38.35	B
ATOM	2367	NH2	ARG	329	23.513	-3.284	49.119	1.00	36.37	B
ATOM	2368	C	ARG	329	23.761	-0.102	56.061	1.00	22.51	B
ATOM	2369	O	ARG	329	24.174	1.012	55.741	1.00	21.91	B
ATOM	2370	N	THR	330	24.431	-0.919	56.856	1.00	21.40	B
ATOM	2371	CA	THR	330	25.704	-0.529	57.433	1.00	21.18	B
ATOM	2372	CB	THR	330	25.610	-0.435	58.971	1.00	20.58	B
ATOM	2373	OG1	THR	330	24.666	0.581	59.317	1.00	22.60	B
ATOM	2374	CG2	THR	330	26.962	-0.099	59.581	1.00	17.89	B
ATOM	2375	C	THR	330	26.837	-1.471	57.085	1.00	21.32	B
ATOM	2376	O	THR	330	26.673	-2.691	57.001	1.00	19.41	B
ATOM	2377	N	SER	331	28.002	-0.872	56.902	1.00	21.49	B
ATOM	2378	CA	SER	331	29.200	-1.602	56.574	1.00	21.39	B
ATOM	2379	CB	SER	331	29.469	-1.473	55.084	1.00	22.34	B
ATOM	2380	OG	SER	331	30.537	-2.313	54.694	1.00	26.49	B
ATOM	2381	C	SER	331	30.340	-1.001	57.391	1.00	20.49	B
ATOM	2382	O	SER	331	30.418	0.208	57.565	1.00	21.48	B
ATOM	2383	N	ILE	332	31.213	-1.849	57.911	1.00	18.89	B
ATOM	2384	CA	ILE	332	32.341	-1.371	58.695	1.00	15.95	B
ATOM	2385	CB	ILE	332	32.321	-1.936	60.135	1.00	15.17	B
ATOM	2386	CG2	ILE	332	33.621	-1.568	60.854	1.00	12.52	B
ATOM	2387	CG1	ILE	332	31.091	-1.447	60.882	1.00	11.58	B
ATOM	2388	CD1	ILE	332	30.932	-2.097	62.247	1.00	7.00	B
ATOM	2389	C	ILE	332	33.650	-1.818	58.063	1.00	15.41	B
ATOM	2390	O	ILE	332	33.802	-2.980	57.687	1.00	12.48	B
ATOM	2391	N	ILE	333	34.591	-0.888	57.948	1.00	16.21	B
ATOM	2392	CA	ILE	333	35.899	-1.203	57.411	1.00	16.71	B
ATOM	2393	CB	ILE	333	36.310	-0.266	56.273	1.00	16.82	B
ATOM	2394	CG2	ILE	333	37.616	-0.744	55.675	1.00	15.94	B
ATOM	2395	CG1	ILE	333	35.242	-0.259	55.169	1.00	16.68	B
ATOM	2396	CD1	ILE	333	35.557	0.705	54.012	1.00	15.18	B
ATOM	2397	C	ILE	333	36.860	-1.021	58.561	1.00	18.56	B
ATOM	2398	O	ILE	333	37.074	0.104	59.032	1.00	21.41	B
ATOM	2399	N	ALA	334	37.411	-2.137	59.035	1.00	20.14	B
ATOM	2400	CA	ALA	334	38.360	-2.125	60.147	1.00	19.94	B
ATOM	2401	CB	ALA	334	38.182	-3.362	61.020	1.00	18.30	B
ATOM	2402	C	ALA	334	39.756	-2.096	59.550	1.00	20.34	B
ATOM	2403	O	ALA	334	40.135	-2.989	58.790	1.00	20.44	B
ATOM	2404	N	THR	335	40.514	-1.062	59.897	1.00	19.08	B
ATOM	2405	CA	THR	335	41.853	-0.901	59.369	1.00	19.70	B
ATOM	2406	CB	THR	335	42.106	0.584	59.008	1.00	21.15	B
ATOM	2407	OG1	THR	335	41.876	1.409	60.157	1.00	24.31	B
ATOM	2408	CG2	THR	335	41.158	1.026	57.905	1.00	21.90	B
ATOM	2409	C	THR	335	42.907	-1.403	60.351	1.00	19.67	B
ATOM	2410	O	THR	335	42.796	-1.190	61.559	1.00	20.81	B
ATOM	2411	N	ILE	336	43.924	-2.085	59.833	1.00	19.06	B
ATOM	2412	CA	ILE	336	44.991	-2.618	60.680	1.00	19.16	B
ATOM	2413	CB	ILE	336	44.845	-4.147	60.882	1.00	18.20	B
ATOM	2414	CG2	ILE	336	43.519	-4.470	61.562	1.00	17.20	B
ATOM	2415	CG1	ILE	336	44.933	-4.857	59.564	1.00	15.56	B
ATOM	2416	CD1	ILE	336	44.926	-6.371	59.697	1.00	16.09	B
ATOM	2417	C	ILE	336	46.388	-2.343	60.116	1.00	19.85	B
ATOM	2418	O	ILE	336	46.547	-1.995	58.945	1.00	20.63	B
ATOM	2419	N	SER	337	47.395	-2.487	60.970	1.00	21.82	B
ATOM	2420	CA	SER	337	48.788	-2.277	60.576	1.00	23.86	B
ATOM	2421	CB	SER	337	49.514	-1.430	61.611	1.00	22.35	B
ATOM	2422	OG	SER	337	50.551	-2.165	62.229	1.00	19.41	B

ATOM	2423	C	SER	337	49.507	-3.622	60.458	1.00	26.10	B
ATOM	2424	O	SER	337	49.133	-4.597	61.119	1.00	25.43	B
ATOM	2425	N	PRO	338	50.543	-3.692	59.606	1.00	26.45	B
ATOM	2426	CD	PRO	338	50.873	-2.755	58.518	1.00	26.43	B
ATOM	2427	CA	PRO	338	51.287	-4.943	59.441	1.00	27.75	B
ATOM	2428	CB	PRO	338	51.703	-4.893	58.009	1.00	25.91	B
ATOM	2429	CG	PRO	338	52.043	-3.453	57.835	1.00	26.04	B
ATOM	2430	C	PRO	338	52.493	-5.016	60.366	1.00	28.99	B
ATOM	2431	O	PRO	338	53.304	-5.929	60.250	1.00	30.27	B
ATOM	2432	N	ALA	339	52.615	-4.057	61.280	1.00	29.91	B
ATOM	2433	CA	ALA	339	53.765	-4.024	62.184	1.00	31.92	B
ATOM	2434	CB	ALA	339	54.076	-2.582	62.598	1.00	32.09	B
ATOM	2435	C	ALA	339	53.576	-4.884	63.415	1.00	31.91	B
ATOM	2436	O	ALA	339	52.483	-4.965	63.959	1.00	34.29	B
ATOM	2437	N	SER	340	54.651	-5.525	63.856	1.00	31.24	B
ATOM	2438	CA	SER	340	54.580	-6.374	65.030	1.00	29.08	B
ATOM	2439	CB	SER	340	55.877	-7.280	65.138	1.00	29.57	B
ATOM	2440	OG	SER	340	57.053	-6.513	65.327	1.00	28.10	B
ATOM	2441	C	SER	340	54.396	-5.555	66.307	1.00	28.00	B
ATOM	2442	O	SER	340	53.844	-6.046	67.280	1.00	28.20	B
ATOM	2443	N	LEU	341	54.852	-4.308	66.309	1.00	28.24	B
ATOM	2444	CA	LEU	341	54.715	-3.471	67.493	1.00	28.05	B
ATOM	2445	CB	LEU	341	55.742	-2.306	67.463	1.00	29.43	B
ATOM	2446	CG	LEU	341	55.315	-0.861	67.190	1.00	30.31	B
ATOM	2447	CD1	LEU	341	56.404	0.084	67.690	1.00	28.26	B
ATOM	2448	CD2	LEU	341	55.065	-0.659	65.707	1.00	31.94	B
ATOM	2449	C	LEU	341	53.290	-2.936	67.647	1.00	28.81	B
ATOM	2450	O	LEU	341	52.954	-2.305	68.650	1.00	28.00	B
ATOM	2451	N	ASN	342	52.450	-3.209	66.656	1.00	28.88	B
ATOM	2452	CA	ASN	342	51.060	-2.780	66.690	1.00	29.97	B
ATOM	2453	CB	ASN	342	50.689	-2.094	65.369	1.00	28.90	B
ATOM	2454	CG	ASN	342	51.256	-0.680	65.258	1.00	29.29	B
ATOM	2455	OD1	ASN	342	51.568	-0.210	64.161	1.00	27.68	B
ATOM	2456	ND2	ASN	342	51.373	0.007	66.394	1.00	26.96	B
ATOM	2457	C	ASN	342	50.185	-4.010	66.902	1.00	31.53	B
ATOM	2458	O	ASN	342	48.958	-3.956	66.765	1.00	32.86	B
ATOM	2459	N	LEU	343	50.830	-5.118	67.252	1.00	30.95	B
ATOM	2460	CA	LEU	343	50.143	-6.387	67.474	1.00	30.40	B
ATOM	2461	CB	LEU	343	51.167	-7.448	67.961	1.00	31.48	B
ATOM	2462	CG	LEU	343	50.755	-8.930	68.109	1.00	33.60	B
ATOM	2463	CD1	LEU	343	50.408	-9.217	69.553	1.00	34.09	B
ATOM	2464	CD2	LEU	343	49.599	-9.270	67.168	1.00	31.95	B
ATOM	2465	C	LEU	343	48.945	-6.325	68.422	1.00	28.19	B
ATOM	2466	O	LEU	343	47.839	-6.698	68.042	1.00	29.33	B
ATOM	2467	N	GLU	344	49.145	-5.858	69.647	1.00	26.96	B
ATOM	2468	CA	GLU	344	48.035	-5.787	70.598	1.00	25.82	B
ATOM	2469	CB	GLU	344	48.537	-5.276	71.962	1.00	27.56	B
ATOM	2470	CG	GLU	344	47.438	-4.776	72.879	1.00	33.02	B
ATOM	2471	CD	GLU	344	47.884	-4.708	74.329	1.00	36.74	B
ATOM	2472	OE1	GLU	344	49.011	-4.222	74.583	1.00	36.88	B
ATOM	2473	OE2	GLU	344	47.104	-5.138	75.217	1.00	38.52	B
ATOM	2474	C	GLU	344	46.843	-4.948	70.122	1.00	23.12	B
ATOM	2475	O	GLU	344	45.696	-5.357	70.265	1.00	22.53	B
ATOM	2476	N	GLU	345	47.102	-3.775	69.564	1.00	22.13	B
ATOM	2477	CA	GLU	345	46.007	-2.949	69.082	1.00	22.56	B
ATOM	2478	CB	GLU	345	46.484	-1.487	68.830	1.00	23.16	B
ATOM	2479	CG	GLU	345	46.722	-0.693	70.108	1.00	23.64	B
ATOM	2480	CD	GLU	345	45.440	-0.386	70.872	1.00	25.85	B
ATOM	2481	OE1	GLU	345	45.530	0.135	72.003	1.00	29.18	B
ATOM	2482	OE2	GLU	345	44.342	-0.653	70.352	1.00	25.14	B
ATOM	2483	C	GLU	345	45.422	-3.566	67.808	1.00	21.03	B
ATOM	2484	O	GLU	345	44.238	-3.398	67.519	1.00	20.99	B
ATOM	2485	N	THR	346	46.253	-4.274	67.048	1.00	20.57	B
ATOM	2486	CA	THR	346	45.794	-4.959	65.838	1.00	20.75	B
ATOM	2487	CB	THR	346	46.978	-5.579	65.057	1.00	21.69	B
ATOM	2488	OG1	THR	346	47.743	-4.531	64.460	1.00	23.54	B
ATOM	2489	CG2	THR	346	46.486	-6.540	63.964	1.00	20.78	B
ATOM	2490	C	THR	346	44.825	-6.070	66.269	1.00	20.06	B
ATOM	2491	O	THR	346	43.824	-6.323	65.603	1.00	19.82	B
ATOM	2492	N	LEU	347	45.127	-6.717	67.395	1.00	19.28	B
ATOM	2493	CA	LEU	347	44.265	-7.771	67.924	1.00	20.23	B
ATOM	2494	CB	LEU	347	44.967	-8.547	69.080	1.00	20.75	B
ATOM	2495	CG	LEU	347	46.123	-9.517	68.681	1.00	20.74	B

ATOM	2496	CD1	LEU	347	46.659	-10.198	69.923	1.00	18.01	B
ATOM	2497	CD2	LEU	347	45.630	-10.563	67.681	1.00	19.87	B
ATOM	2498	C	LEU	347	42.950	-7.187	68.426	1.00	20.24	B
ATOM	2499	O	LEU	347	41.884	-7.735	68.165	1.00	20.79	B
ATOM	2500	N	SER	348	43.019	-6.074	69.148	1.00	19.68	B
ATOM	2501	CA	SER	348	41.800	-5.450	69.645	1.00	18.65	B
ATOM	2502	CB	SER	348	42.123	-4.205	70.337	1.00	18.12	B
ATOM	2503	OG	SER	348	42.924	-4.491	71.458	1.00	23.16	B
ATOM	2504	C	SER	348	40.848	-5.161	68.498	1.00	18.64	B
ATOM	2505	O	SER	348	39.662	-5.505	68.560	1.00	17.43	B
ATOM	2506	N	THR	349	41.377	-4.535	67.447	1.00	18.49	B
ATOM	2507	CA	THR	349	40.577	-4.195	66.274	1.00	20.04	B
ATOM	2508	CB	THR	349	41.440	-3.523	65.189	1.00	21.24	B
ATOM	2509	OG1	THR	349	41.774	-2.195	65.607	1.00	22.77	B
ATOM	2510	CG2	THR	349	40.692	-3.471	63.848	1.00	20.74	B
ATOM	2511	C	THR	349	39.873	-5.402	65.658	1.00	20.94	B
ATOM	2512	O	THR	349	38.651	-5.399	65.516	1.00	19.02	B
ATOM	2513	N	LEU	350	40.645	-6.423	65.280	1.00	23.75	B
ATOM	2514	CA	LEU	350	40.072	-7.632	64.682	1.00	25.37	B
ATOM	2515	CB	LEU	350	41.155	-8.728	64.483	1.00	24.15	B
ATOM	2516	CG	LEU	350	42.104	-8.768	63.261	1.00	23.69	B
ATOM	2517	CD1	LEU	350	41.548	-7.931	62.146	1.00	24.69	B
ATOM	2518	CD2	LEU	350	43.476	-8.294	63.652	1.00	25.26	B
ATOM	2519	C	LEU	350	38.967	-8.204	65.570	1.00	25.64	B
ATOM	2520	O	LEU	350	37.925	-8.651	65.088	1.00	25.79	B
ATOM	2521	N	GLU	351	39.215	-8.179	66.873	1.00	26.21	B
ATOM	2522	CA	GLU	351	38.280	-8.705	67.859	1.00	26.22	B
ATOM	2523	CB	GLU	351	38.950	-8.729	69.230	1.00	29.30	B
ATOM	2524	CG	GLU	351	38.325	-9.722	70.181	1.00	35.95	B
ATOM	2525	CD	GLU	351	38.148	-11.081	69.528	1.00	39.86	B
ATOM	2526	OE1	GLU	351	39.180	-11.726	69.204	1.00	39.55	B
ATOM	2527	OE2	GLU	351	36.973	-11.484	69.326	1.00	40.87	B
ATOM	2528	C	GLU	351	36.995	-7.887	67.927	1.00	24.59	B
ATOM	2529	O	GLU	351	35.886	-8.438	67.987	1.00	24.44	B
ATOM	2530	N	TYR	352	37.163	-6.569	67.922	1.00	22.44	B
ATOM	2531	CA	TYR	352	36.058	-5.627	67.973	1.00	20.05	B
ATOM	2532	CB	TYR	352	36.638	-4.176	68.166	1.00	20.78	B
ATOM	2533	CG	TYR	352	35.618	-3.065	68.285	1.00	19.34	B
ATOM	2534	CD1	TYR	352	34.997	-2.539	67.153	1.00	17.81	B
ATOM	2535	CE1	TYR	352	34.062	-1.515	67.258	1.00	19.71	B
ATOM	2536	CD2	TYR	352	35.277	-2.535	69.533	1.00	19.30	B
ATOM	2537	CE2	TYR	352	34.339	-1.507	69.649	1.00	17.88	B
ATOM	2538	CZ	TYR	352	33.737	-1.003	68.508	1.00	19.50	B
ATOM	2539	OH	TYR	352	32.810	0.017	68.602	1.00	23.10	B
ATOM	2540	C	TYR	352	35.211	-5.723	66.706	1.00	20.25	B
ATOM	2541	O	TYR	352	33.989	-5.704	66.776	1.00	20.39	B
ATOM	2542	N	ALA	353	35.855	-5.851	65.549	1.00	20.55	B
ATOM	2543	CA	ALA	353	35.122	-5.941	64.289	1.00	23.02	B
ATOM	2544	CB	ALA	353	36.076	-5.711	63.116	1.00	20.71	B
ATOM	2545	C	ALA	353	34.374	-7.271	64.109	1.00	25.05	B
ATOM	2546	O	ALA	353	33.259	-7.299	63.580	1.00	24.67	B
ATOM	2547	N	HIS	354	34.983	-8.366	64.553	1.00	26.56	B
ATOM	2548	CA	HIS	354	34.372	-9.682	64.420	1.00	29.08	B
ATOM	2549	CB	HIS	354	35.332	-10.761	64.917	1.00	30.47	B
ATOM	2550	CG	HIS	354	34.916	-12.150	64.547	1.00	31.52	B
ATOM	2551	CD2	HIS	354	34.400	-13.156	65.293	1.00	30.23	B
ATOM	2552	ND1	HIS	354	34.990	-12.629	63.255	1.00	32.72	B
ATOM	2553	CE1	HIS	354	34.539	-13.870	63.222	1.00	32.65	B
ATOM	2554	NE2	HIS	354	34.175	-14.213	64.445	1.00	32.59	B
ATOM	2555	C	HIS	354	33.059	-9.754	65.194	1.00	30.20	B
ATOM	2556	O	HIS	354	32.075	-10.332	64.722	1.00	30.57	B
ATOM	2557	N	ARG	355	33.044	-9.177	66.390	1.00	31.47	B
ATOM	2558	CA	ARG	355	31.825	-9.166	67.182	1.00	33.23	B
ATOM	2559	CB	ARG	355	32.064	-8.504	68.551	1.00	35.96	B
ATOM	2560	CG	ARG	355	32.853	-9.364	69.516	1.00	40.08	B
ATOM	2561	CD	ARG	355	33.214	-8.625	70.797	1.00	43.24	B
ATOM	2562	NE	ARG	355	32.052	-8.198	71.579	1.00	47.90	B
ATOM	2563	CZ	ARG	355	31.127	-9.016	72.081	1.00	50.90	B
ATOM	2564	NH1	ARG	355	31.208	-10.329	71.881	1.00	50.97	B
ATOM	2565	NH2	ARG	355	30.128	-8.521	72.806	1.00	50.14	B
ATOM	2566	C	ARG	355	30.770	-8.378	66.413	1.00	32.60	B
ATOM	2567	O	ARG	355	29.619	-8.801	66.321	1.00	32.82	B
ATOM	2568	N	ALA	356	31.178	-7.240	65.850	1.00	29.87	B

ATOM	2569	CA	ALA	356	30.266	-6.389	65.096	1.00	27.94	B
ATOM	2570	CB	ALA	356	31.025	-5.243	64.467	1.00	28.16	B
ATOM	2571	C	ALA	356	29.485	-7.137	64.022	1.00	26.92	B
ATOM	2572	O	ALA	356	28.356	-6.759	63.698	1.00	24.79	B
ATOM	2573	N	LYS	357	30.074	-8.203	63.486	1.00	25.84	B
ATOM	2574	CA	LYS	357	29.416	-8.982	62.438	1.00	27.17	B
ATOM	2575	CB	LYS	357	30.248	-10.193	62.040	1.00	26.83	B
ATOM	2576	CG	LYS	357	31.690	-9.905	61.724	1.00	28.45	B
ATOM	2577	CD	LYS	357	32.191	-10.857	60.651	1.00	31.56	B
ATOM	2578	CE	LYS	357	31.933	-12.305	61.008	1.00	31.36	B
ATOM	2579	NZ	LYS	357	32.361	-13.190	59.908	1.00	30.37	B
ATOM	2580	C	LYS	357	28.036	-9.483	62.831	1.00	27.51	B
ATOM	2581	O	LYS	357	27.173	-9.651	61.974	1.00	27.57	B
ATOM	2582	N	ASN	358	27.829	-9.728	64.121	1.00	28.92	B
ATOM	2583	CA	ASN	358	26.546	-10.234	64.597	1.00	30.60	B
ATOM	2584	CB	ASN	358	26.741	-11.024	65.911	1.00	31.34	B
ATOM	2585	CG	ASN	358	27.527	-12.311	65.709	1.00	33.50	B
ATOM	2586	OD1	ASN	358	28.750	-12.292	65.537	1.00	34.98	B
ATOM	2587	ND2	ASN	358	26.823	-13.439	65.716	1.00	33.36	B
ATOM	2588	C	ASN	358	25.426	-9.207	64.788	1.00	30.89	B
ATOM	2589	O	ASN	358	24.367	-9.547	65.302	1.00	32.42	B
ATOM	2590	N	ILE	359	25.642	-7.961	64.381	1.00	31.36	B
ATOM	2591	CA	ILE	359	24.607	-6.943	64.530	1.00	31.09	B
ATOM	2592	CB	ILE	359	25.185	-5.505	64.454	1.00	30.83	B
ATOM	2593	CG2	ILE	359	24.060	-4.493	64.496	1.00	28.14	B
ATOM	2594	CG1	ILE	359	26.144	-5.246	65.629	1.00	29.88	B
ATOM	2595	CD1	ILE	359	27.028	-4.031	65.421	1.00	29.12	B
ATOM	2596	C	ILE	359	23.583	-7.110	63.416	1.00	32.70	B
ATOM	2597	O	ILE	359	23.938	-7.293	62.250	1.00	31.89	B
ATOM	2598	N	LEU	360	22.312	-7.045	63.795	1.00	34.93	B
ATOM	2599	CA	LEU	360	21.195	-7.185	62.869	1.00	37.63	B
ATOM	2600	CB	LEU	360	20.056	-7.993	63.544	1.00	39.00	B
ATOM	2601	CG	LEU	360	18.581	-7.590	63.189	1.00	41.16	B
ATOM	2602	CD1	LEU	360	18.283	-7.917	61.728	1.00	42.20	B
ATOM	2603	CD2	LEU	360	17.599	-8.315	64.118	1.00	41.50	B
ATOM	2604	C	LEU	360	20.672	-5.814	62.475	1.00	38.26	B
ATOM	2605	O	LEU	360	20.356	-5.003	63.343	1.00	38.46	B
ATOM	2606	N	ASN	361	20.580	-5.565	61.171	1.00	39.80	B
ATOM	2607	CA	ASN	361	20.079	-4.295	60.656	1.00	41.76	B
ATOM	2608	CB	ASN	361	21.133	-3.606	59.822	1.00	42.66	B
ATOM	2609	CG	ASN	361	22.088	-2.772	60.657	1.00	44.51	B
ATOM	2610	OD1	ASN	361	22.791	-3.289	61.528	1.00	45.27	B
ATOM	2611	ND2	ASN	361	22.117	-1.467	60.394	1.00	45.23	B
ATOM	2612	C	ASN	361	18.825	-4.481	59.812	1.00	44.12	B
ATOM	2613	O	ASN	361	18.478	-5.604	59.438	1.00	45.59	B
ATOM	2614	N	LYS	362	18.160	-3.366	59.514	1.00	45.40	B
ATOM	2615	CA	LYS	362	16.931	-3.332	58.716	1.00	45.80	B
ATOM	2616	CB	LYS	362	17.226	-3.756	57.260	1.00	45.62	B
ATOM	2617	CG	LYS	362	17.222	-2.619	56.240	1.00	45.92	B
ATOM	2618	CD	LYS	362	15.832	-2.001	56.093	1.00	45.58	B
ATOM	2619	CE	LYS	362	15.739	-1.104	54.862	1.00	43.34	B
ATOM	2620	NZ	LYS	362	14.456	-0.345	54.818	1.00	42.49	B
ATOM	2621	C	LYS	362	15.823	-4.213	59.292	1.00	47.03	B
ATOM	2622	O	LYS	362	15.150	-4.897	58.492	1.00	48.78	B
ATOM	2623	OXT	LYS	362	15.624	-4.198	60.526	1.00	47.26	B
ATOM	2624	MG	MG	2602	43.330	10.372	60.103	1.00	26.54	
ATOM	2625	PB	ADP	2600	44.452	7.135	60.400	1.00	17.43	ADP
ATOM	2626	O1B	ADP	2600	44.951	7.845	61.612	1.00	18.86	ADP
ATOM	2627	O2B	ADP	2600	44.008	5.637	60.747	1.00	22.98	ADP
ATOM	2628	O3B	ADP	2600	43.299	7.848	59.790	1.00	19.76	ADP
ATOM	2629	PA	ADP	2600	45.880	7.608	57.967	1.00	24.97	ADP
ATOM	2630	O1A	ADP	2600	44.906	7.153	56.989	1.00	27.54	ADP
ATOM	2631	O2A	ADP	2600	45.805	9.067	58.061	1.00	29.40	ADP
ATOM	2632	O3A	ADP	2600	45.606	6.967	59.369	1.00	22.28	ADP
ATOM	2633	O5*	ADP	2600	47.347	7.314	57.518	1.00	28.31	ADP
ATOM	2634	C5*	ADP	2600	48.422	6.620	58.144	1.00	30.71	ADP
ATOM	2635	C4*	ADP	2600	49.601	6.747	57.103	1.00	33.98	ADP
ATOM	2636	O4*	ADP	2600	49.664	5.485	56.457	1.00	33.98	ADP
ATOM	2637	C3*	ADP	2600	49.383	7.792	55.972	1.00	32.52	ADP
ATOM	2638	O3*	ADP	2600	50.518	8.657	55.838	1.00	36.94	ADP
ATOM	2639	C2*	ADP	2600	49.106	7.017	54.682	1.00	35.49	ADP
ATOM	2640	O2*	ADP	2600	49.782	7.556	53.522	1.00	38.23	ADP
ATOM	2641	C1*	ADP	2600	49.483	5.577	55.026	1.00	35.20	ADP

ATOM	2642	N9	ADP	2600	48.437	4.548	54.689	1.00	33.78		ADP
ATOM	2643	C8	ADP	2600	47.512	4.099	55.567	1.00	34.18		ADP
ATOM	2644	N7	ADP	2600	46.745	3.202	55.003	1.00	36.36		ADP
ATOM	2645	C5	ADP	2600	47.137	3.045	53.768	1.00	36.94		ADP
ATOM	2646	C6	ADP	2600	46.721	2.241	52.700	1.00	37.31		ADP
ATOM	2647	N6	ADP	2600	45.687	1.403	52.874	1.00	37.72		ADP
ATOM	2648	N1	ADP	2600	47.381	2.320	51.471	1.00	37.39		ADP
ATOM	2649	C2	ADP	2600	48.446	3.171	51.268	1.00	37.76		ADP
ATOM	2650	N3	ADP	2600	48.859	3.957	52.311	1.00	35.88		ADP
ATOM	2651	C4	ADP	2600	48.245	3.925	53.548	1.00	35.51		ADP
ATOM	2652	C1	1-7	1	37.929	17.272	54.077	1.00	38.43		1-7
ATOM	2653	C2	1-7	1	38.932	17.045	53.074	1.00	38.52		1-7
ATOM	2654	C3	1-7	1	38.735	15.932	52.163	1.00	39.96		1-7
ATOM	2655	C4	1-7	1	37.528	15.091	52.280	1.00	39.17		1-7
ATOM	2656	C5	1-7	1	36.503	15.314	53.268	1.00	37.92		1-7
ATOM	2657	C6	1-7	1	36.737	16.421	54.166	1.00	39.95		1-7
ATOM	2658	C11	1-7	1	39.781	15.680	51.154	1.00	38.83		1-7
ATOM	2659	N12	1-7	1	40.860	16.465	50.816	1.00	41.41		1-7
ATOM	2660	N13	1-7	1	41.632	15.978	49.912	1.00	42.37		1-7
ATOM	2661	C14	1-7	1	41.128	14.690	49.355	1.00	40.44		1-7
ATOM	2662	C15	1-7	1	40.183	14.416	50.455	1.00	39.39		1-7
ATOM	2663	C18	1-7	1	41.056	14.226	47.951	1.00	36.95		1-7
ATOM	2664	C20	1-7	1	42.809	16.554	49.520	1.00	43.23		1-7
ATOM	2665	C21	1-7	1	43.706	15.596	48.761	1.00	42.51		1-7
ATOM	2666	O25	1-7	1	43.145	17.720	49.767	1.00	44.94		1-7
ATOM	2667	C26	1-7	1	40.067	14.828	47.075	1.00	35.46		1-7
ATOM	2668	C27	1-7	1	40.008	14.513	45.661	1.00	35.09		1-7
ATOM	2669	C28	1-7	1	40.989	13.573	45.157	1.00	34.04		1-7
ATOM	2670	C29	1-7	1	41.984	12.977	46.048	1.00	34.13		1-7
ATOM	2671	C30	1-7	1	42.012	13.263	47.467	1.00	34.81		1-7
ATOM	2672	CL35	1-7	1	37.356	13.776	51.201	1.00	40.06		1-7
ATOM	2673	O36	1-7	1	42.983	12.166	45.535	1.00	32.08		1-7
ATOM	2674	O	HOH	2	38.525	10.810	62.766	1.00	2.98		S
ATOM	2675	O	HOH	3	23.222	11.589	60.100	1.00	22.29		S
ATOM	2676	O	HOH	4	41.960	12.208	60.870	1.00	9.69		S
ATOM	2677	O	HOH	5	50.029	-4.994	63.682	1.00	18.21		S
ATOM	2678	O	HOH	8	28.413	21.060	56.800	1.00	20.56		S
ATOM	2679	O	HOH	9	31.397	6.826	80.114	1.00	18.48		S
ATOM	2680	O	HOH	10	38.337	3.375	65.490	1.00	21.12		S
ATOM	2681	O	HOH	13	45.628	22.010	69.140	1.00	9.64		S
ATOM	2682	O	HOH	14	48.257	14.330	41.733	1.00	18.62		S
ATOM	2683	O	HOH	15	41.014	5.558	71.890	1.00	28.07		S
ATOM	2684	O	HOH	16	27.936	20.868	70.581	1.00	22.56		S
ATOM	2685	O	HOH	17	43.663	-1.056	64.226	1.00	13.66		S
ATOM	2686	O	HOH	18	43.194	8.354	64.240	1.00	19.73		S
ATOM	2687	O	HOH	20	54.924	6.098	49.933	1.00	32.18		S
ATOM	2688	O	HOH	22	31.350	4.322	82.668	1.00	37.14		S
ATOM	2689	O	HOH	27	45.521	-1.603	51.520	1.00	20.22		S
ATOM	2690	O	HOH	28	53.208	11.559	41.772	1.00	42.11		S
ATOM	2691	O	HOH	31	27.994	6.504	79.871	1.00	18.94		S
ATOM	2692	O	HOH	33	49.291	-7.879	50.486	1.00	35.78		S
ATOM	2693	O	HOH	34	18.468	12.203	33.372	1.00	19.62		S
ATOM	2694	O	HOH	35	53.496	-17.951	61.642	1.00	35.98		S
ATOM	2695	O	HOH	36	45.680	3.185	45.465	1.00	19.30		S
ATOM	2696	O	HOH	38	42.176	-0.846	72.113	1.00	14.70		S
ATOM	2697	O	HOH	39	51.304	5.232	60.441	1.00	24.96		S
ATOM	2698	O	HOH	40	34.806	13.087	70.806	1.00	32.37		S
ATOM	2699	O	HOH	41	19.156	14.294	56.441	1.00	28.63		S
ATOM	2700	O	HOH	46	44.126	0.351	55.876	1.00	28.55		S
ATOM	2701	O	HOH	47	20.432	7.836	62.530	1.00	16.12		S
ATOM	2702	O	HOH	48	31.643	24.934	63.575	1.00	31.65		S
ATOM	2703	O	HOH	50	45.290	17.359	64.325	1.00	15.86		S
ATOM	2704	O	HOH	53	41.790	5.942	40.546	1.00	28.37		S
ATOM	2705	O	HOH	54	38.452	4.419	47.214	1.00	14.56		S
ATOM	2706	O	HOH	55	52.009	4.613	57.096	1.00	35.87		S
ATOM	2707	O	HOH	57	51.429	6.864	39.244	1.00	27.91		S
ATOM	2708	O	HOH	58	22.685	19.136	43.047	1.00	29.36		S
ATOM	2709	O	HOH	61	39.044	12.519	58.483	1.00	28.94		S
ATOM	2710	O	HOH	67	45.314	-7.264	72.406	1.00	17.23		S
ATOM	2711	O	HOH	69	46.768	-2.040	64.134	1.00	23.58		S
ATOM	2712	O	HOH	71	45.298	18.821	48.751	1.00	30.98		S
ATOM	2713	O	HOH	79	45.903	11.457	63.308	1.00	21.87		S
ATOM	2714	O	HOH	83	29.506	-5.557	49.394	1.00	32.50		S

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ATOM   2715  O   HOH    86      28.178   4.602  77.098  1.00 29.04      S
ATOM   2716  O   HOH    89      55.210 -16.662  58.167  1.00 35.61      S
ATOM   2717  O   HOH    91      37.135   0.846  70.878  1.00 20.52      S
ATOM   2718  O   HOH    93      17.438  19.816  52.756  1.00 35.47      S
ATOM   2719  O   HOH    94      29.881   3.798  41.417  1.00 42.97      S
ATOM   2720  O   HOH    98      39.190   3.892  49.946  1.00 13.01      S
ATOM   2721  O   HOH   100      41.671  15.312  56.323  1.00 31.21      S
ATOM   2722  O   HOH   101      52.876   0.835  68.812  1.00 32.79      S
ATOM   2723  O   HOH   105      37.722   2.513  73.490  1.00 36.02      S
ATOM   2724  O   HOH   109      27.450  25.927  61.040  1.00 42.15      S
ATOM   2725  O   HOH   111      39.804  17.000  76.527  1.00 40.03      S
ATOM   2726  O   HOH   117       2.532   6.263  36.270  1.00 22.77      S
ATOM   2727  O   HOH   119      43.756   2.932  43.574  1.00 30.63      S
ATOM   2728  O   HOH   124      41.324   9.248  61.513  1.00 50.60      S
ATOM   2729  O   HOH   128      45.349  21.055  46.092  1.00 34.28      S
ATOM   2730  O   HOH   129      47.480   9.402  61.725  1.00 20.53      S
ATOM   2731  O   HOH   130      27.022  14.663  58.188  1.00 21.56      S
ATOM   2732  O   HOH   131      38.009  11.637  34.970  1.00 36.04      S
ATOM   2733  O   HOH   135      21.462  18.078  39.253  1.00 49.42      S
ATOM   2734  O   HOH   136      50.206  -0.381  68.977  1.00 28.73      S
ATOM   2735  O   HOH   142      43.209  19.312  57.176  1.00 32.90      S
ATOM   2736  O   HOH   144      27.420 -13.840  56.585  1.00 40.61      S
ATOM   2737  O   HOH   145      56.085   3.298  61.538  1.00 27.46      S
ATOM   2738  O   HOH   148      45.044  22.181  54.899  1.00 33.67      S
ATOM   2739  O   HOH   149      47.168   9.785  68.295  1.00 32.20      S
ATOM   2740  O   HOH   150      35.221  13.107  56.556  1.00 39.71      S
ATOM   2741  O   HOH   156      19.494  13.147  35.697  1.00 37.79      S
ATOM   2742  O   HOH   158      35.348   1.853  79.606  1.00 35.97      S
ATOM   2743  O   HOH   160      44.086  -3.335  73.582  1.00 28.68      S
ATOM   2744  O   HOH   163      22.716  28.692  55.723  1.00 38.12      S
ATOM   2745  O   HOH   164      29.077  26.837  62.948  1.00 37.04      S
END
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TABLE 3

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 REMARK refinement resolution: 50.0 - 2.5 A
REMARK final     r= 0.2461 free_r= 0.3007
REMARK rmsd bonds= 0.007673  rmsd angles=  1.23268
REMARK sg= P2(1)2(1)2(1) a= 68.9 b= 79.4 c= 158.8 alpha= 90. beta= 90. gamma= 90.
REMARK FILENAME="Compound 2-7_3pb.pdb"
ATOM      1  CB  LYS    17      24.357 -12.099  59.933  1.00 58.09      B
ATOM      2  CG  LYS    17      23.017 -12.631  59.411  1.00 60.84      B
ATOM      3  CD  LYS    17      22.865 -12.482  57.896  1.00 62.11      B
ATOM      4  CE  LYS    17      23.604 -13.578  57.123  1.00 63.01      B
ATOM      5  NZ  LYS    17      25.089 -13.550  57.289  1.00 63.35      B
ATOM      6  C   LYS    17      24.262  -9.737  59.096  1.00 54.65      B
ATOM      7  O   LYS    17      25.150  -9.723  58.262  1.00 53.83      B
ATOM      8  N   LYS    17      23.253 -10.341  61.285  1.00 56.25      B
ATOM      9  CA  LYS    17      24.364 -10.617  60.333  1.00 55.82      B
ATOM     10  N   ASN    18      23.168  -8.993  58.994  1.00 53.57      B
ATOM     11  CA  ASN    18      22.956  -8.115  57.857  1.00 52.96      B
ATOM     12  CB  ASN    18      21.634  -7.362  58.018  1.00 55.67      B
ATOM     13  CG  ASN    18      20.433  -8.197  57.613  1.00 58.59      B
ATOM     14  OD1 ASN    18      20.173  -9.261  58.187  1.00 59.98      B
ATOM     15  ND2 ASN    18      19.688  -7.717  56.621  1.00 58.01      B
ATOM     16  C   ASN    18      24.093  -7.115  57.635  1.00 51.27      B
ATOM     17  O   ASN    18      24.391  -6.754  56.495  1.00 52.49      B
ATOM     18  N   ILE    19      24.723  -6.665  58.716  1.00 47.11      B
ATOM     19  CA  ILE    19      25.811  -5.698  58.613  1.00 42.06      B
ATOM     20  CB  ILE    19      26.192  -5.152  60.004  1.00 42.31      B
ATOM     21  CG2 ILE    19      26.598  -6.295  60.917  1.00 43.22      B
ATOM     22  CG1 ILE    19      27.343  -4.159  59.881  1.00 41.90      B
ATOM     23  CD1 ILE    19      27.762  -3.556  61.193  1.00 43.78      B
ATOM     24  C   ILE    19      27.054  -6.300  57.958  1.00 38.26      B
ATOM     25  O   ILE    19      27.480  -7.376  58.312  1.00 38.23      B
ATOM     26  N   GLN    20      27.627  -5.577  56.999  1.00 34.90      B
ATOM     27  CA  GLN    20      28.820  -6.021  56.279  1.00 30.15      B
ATOM     28  CB  GLN    20      28.778  -5.516  54.838  1.00 27.85      B
ATOM     29  CG  GLN    20      30.034  -5.802  54.038  1.00 26.74      B
ATOM     30  CD  GLN    20      29.987  -5.186  52.643  1.00 27.60      B
ATOM     31  OE1 GLN    20      30.137  -3.984  52.484  1.00 29.30      B
ATOM     32  NE2 GLN    20      29.774  -6.017  51.632  1.00 26.15      B
ATOM     33  C   GLN    20      30.091  -5.507  56.949  1.00 29.28      B
ATOM     34  O   GLN    20      30.186  -4.346  57.290  1.00 29.19      B
ATOM     35  N   VAL    21      31.075  -6.379  57.127  1.00 27.08      B
ATOM     36  CA  VAL    21      32.325  -5.975  57.754  1.00 24.84      B
ATOM     37  CB  VAL    21      32.448  -6.546  59.180  1.00 24.84      B
ATOM     38  CG1 VAL    21      33.766  -6.123  59.804  1.00 23.30      B
ATOM     39  CG2 VAL    21      31.274  -6.078  60.033  1.00 24.09      B
ATOM     40  C   VAL    21      33.524  -6.439  56.938  1.00 24.57      B
ATOM     41  O   VAL    21      33.677  -7.608  56.687  1.00 24.54      B
ATOM     42  N   VAL    22      34.370  -5.496  56.531  1.00 25.16      B
ATOM     43  CA  VAL    22      35.558  -5.818  55.753  1.00 24.51      B
ATOM     44  CB  VAL    22      35.493  -5.171  54.356  1.00 25.74      B
ATOM     45  CG1 VAL    22      34.274  -5.694  53.602  1.00 23.07      B
ATOM     46  CG2 VAL    22      35.428  -3.648  54.488  1.00 26.13      B
ATOM     47  C   VAL    22      36.825  -5.350  56.464  1.00 24.25      B
ATOM     48  O   VAL    22      36.769  -4.532  57.376  1.00 25.41      B
ATOM     49  N   VAL    23      37.964  -5.889  56.047  1.00 21.62      B
ATOM     50  CA  VAL    23      39.249  -5.541  56.640  1.00 20.21      B
ATOM     51  CB  VAL    23      39.875  -6.749  57.398  1.00 19.81      B
ATOM     52  CG1 VAL    23      41.246  -6.386  57.920  1.00 17.77      B
ATOM     53  CG2 VAL    23      38.980  -7.164  58.552  1.00 19.57      B
ATOM     54  C   VAL    23      40.224  -5.069  55.565  1.00 20.21      B
ATOM     55  O   VAL    23      40.231  -5.587  54.453  1.00 18.34      B
ATOM     56  N   ARG    24      41.026  -4.063  55.908  1.00 20.97      B
ATOM     57  CA  ARG    24      42.012  -3.508  54.987  1.00 23.76      B
ATOM     58  CB  ARG    24      41.493  -2.221  54.341  1.00 19.71      B
ATOM     59  CG  ARG    24      42.364  -1.729  53.201  1.00 19.19      B
ATOM     60  CD  ARG    24      42.064  -0.294  52.784  1.00 17.94      B
ATOM     61  NE  ARG    24      42.664   0.010  51.487  1.00 16.57      B
ATOM     62  CZ  ARG    24      42.479   1.134  50.801  1.00 18.90      B
ATOM     63  NH1 ARG    24      41.704   2.100  51.281  1.00 16.81      B
ATOM     64  NH2 ARG    24      43.057   1.275  49.615  1.00 16.05      B
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ATOM	65	C	ARG	24	43.304	-3.210	55.736	1.00	27.05	B
ATOM	66	O	ARG	24	43.313	-2.442	56.712	1.00	27.85	B
ATOM	67	N	CYS	25	44.392	-3.820	55.274	1.00	29.51	B
ATOM	68	CA	CYS	25	45.699	-3.637	55.890	1.00	32.32	B
ATOM	69	CB	CYS	25	46.410	-4.991	56.027	1.00	30.86	B
ATOM	70	SG	CYS	25	48.111	-4.890	56.627	1.00	32.54	B
ATOM	71	C	CYS	25	46.545	-2.696	55.045	1.00	33.84	B
ATOM	72	O	CYS	25	46.587	-2.820	53.831	1.00	35.92	B
ATOM	73	N	ARG	26	47.218	-1.754	55.694	1.00	34.94	B
ATOM	74	CA	ARG	26	48.053	-0.807	54.967	1.00	37.11	B
ATOM	75	CB	ARG	26	48.130	0.526	55.723	1.00	37.77	B
ATOM	76	CG	ARG	26	48.388	0.384	57.222	1.00	37.85	B
ATOM	77	CD	ARG	26	49.107	1.591	57.802	1.00	36.08	B
ATOM	78	NE	ARG	26	50.554	1.433	57.704	1.00	35.38	B
ATOM	79	CZ	ARG	26	51.379	1.390	58.747	1.00	35.56	B
ATOM	80	NH1	ARG	26	50.910	1.502	59.982	1.00	32.33	B
ATOM	81	NH2	ARG	26	52.677	1.209	58.551	1.00	37.10	B
ATOM	82	C	ARG	26	49.463	-1.341	54.751	1.00	38.55	B
ATOM	83	O	ARG	26	49.917	-2.224	55.460	1.00	38.07	B
ATOM	84	N	PRO	27	50.170	-0.806	53.752	1.00	40.05	B
ATOM	85	CD	PRO	27	49.674	0.092	52.693	1.00	41.26	B
ATOM	86	CA	PRO	27	51.536	-1.244	53.467	1.00	42.07	B
ATOM	87	CB	PRO	27	51.734	-0.805	52.021	1.00	42.46	B
ATOM	88	CG	PRO	27	50.945	0.468	51.961	1.00	41.54	B
ATOM	89	C	PRO	27	52.508	-0.555	54.418	1.00	43.29	B
ATOM	90	O	PRO	27	52.115	0.329	55.170	1.00	43.49	B
ATOM	91	N	PHE	28	53.773	-0.968	54.380	1.00	45.76	B
ATOM	92	CA	PHE	28	54.807	-0.381	55.233	1.00	47.49	B
ATOM	93	CB	PHE	28	56.045	-1.290	55.308	1.00	46.30	B
ATOM	94	CG	PHE	28	55.770	-2.659	55.861	1.00	45.96	B
ATOM	95	CD1	PHE	28	55.424	-3.709	55.015	1.00	45.49	B
ATOM	96	CD2	PHE	28	55.849	-2.899	57.230	1.00	45.19	B
ATOM	97	CE1	PHE	28	55.162	-4.976	55.526	1.00	44.86	B
ATOM	98	CE2	PHE	28	55.588	-4.165	57.751	1.00	44.92	B
ATOM	99	CZ	PHE	28	55.244	-5.204	56.897	1.00	43.96	B
ATOM	100	C	PHE	28	55.240	0.974	54.686	1.00	49.68	B
ATOM	101	O	PHE	28	55.458	1.127	53.484	1.00	50.76	B
ATOM	102	N	ASN	29	55.369	1.955	55.572	1.00	51.78	B
ATOM	103	CA	ASN	29	55.791	3.289	55.164	1.00	53.98	B
ATOM	104	CB	ASN	29	55.477	4.303	56.268	1.00	52.37	B
ATOM	105	CG	ASN	29	55.889	3.818	57.647	1.00	51.95	B
ATOM	106	OD1	ASN	29	57.068	3.614	57.918	1.00	51.68	B
ATOM	107	ND2	ASN	29	54.909	3.633	58.526	1.00	50.23	B
ATOM	108	C	ASN	29	57.285	3.275	54.841	1.00	56.89	B
ATOM	109	O	ASN	29	57.973	2.293	55.111	1.00	57.68	B
ATOM	110	N	LEU	30	57.779	4.361	54.257	1.00	59.05	B
ATOM	111	CA	LEU	30	59.185	4.452	53.882	1.00	60.93	B
ATOM	112	CB	LEU	30	59.466	5.837	53.293	1.00	60.81	B
ATOM	113	CG	LEU	30	60.555	5.909	52.218	1.00	61.25	B
ATOM	114	CD1	LEU	30	60.401	7.199	51.429	1.00	61.39	B
ATOM	115	CD2	LEU	30	61.935	5.810	52.856	1.00	61.13	B
ATOM	116	C	LEU	30	60.136	4.167	55.047	1.00	62.80	B
ATOM	117	O	LEU	30	61.206	3.611	54.852	1.00	63.36	B
ATOM	118	N	ALA	31	59.736	4.545	56.257	1.00	64.56	B
ATOM	119	CA	ALA	31	60.565	4.326	57.440	1.00	66.24	B
ATOM	120	CB	ALA	31	59.999	5.104	58.617	1.00	64.93	B
ATOM	121	C	ALA	31	60.671	2.846	57.798	1.00	68.38	B
ATOM	122	O	ALA	31	61.757	2.345	58.088	1.00	69.26	B
ATOM	123	N	GLU	32	59.537	2.153	57.781	1.00	69.84	B
ATOM	124	CA	GLU	32	59.492	0.734	58.107	1.00	71.88	B
ATOM	125	CB	GLU	32	58.038	0.275	58.225	1.00	70.67	B
ATOM	126	CG	GLU	32	57.338	0.752	59.487	1.00	67.99	B
ATOM	127	CD	GLU	32	55.831	0.607	59.412	1.00	65.98	B
ATOM	128	OE1	GLU	32	55.174	0.723	60.468	1.00	65.36	B
ATOM	129	OE2	GLU	32	55.302	0.383	58.301	1.00	62.48	B
ATOM	130	C	GLU	32	60.232	-0.143	57.097	1.00	74.40	B
ATOM	131	O	GLU	32	61.090	-0.930	57.472	1.00	74.92	B
ATOM	132	N	ARG	33	59.897	-0.008	55.816	1.00	76.35	B
ATOM	133	CA	ARG	33	60.550	-0.803	54.779	1.00	78.32	B
ATOM	134	CB	ARG	33	59.936	-0.502	53.407	1.00	79.77	B
ATOM	135	CG	ARG	33	59.972	0.964	53.010	1.00	83.18	B
ATOM	136	CD	ARG	33	59.329	1.183	51.645	1.00	85.46	B
ATOM	137	NE	ARG	33	60.032	0.459	50.589	1.00	87.40	B

ATOM	138	CZ	ARG	33	61.269	0.737	50.186	1.00	88.75	B
ATOM	139	NH1	ARG	33	61.948	1.729	50.747	1.00	89.79	B
ATOM	140	NH2	ARG	33	61.828	0.019	49.221	1.00	89.07	B
ATOM	141	C	ARG	33	62.053	-0.536	54.754	1.00	78.80	B
ATOM	142	O	ARG	33	62.832	-1.379	54.318	1.00	78.36	B
ATOM	143	N	LYS	34	62.448	0.644	55.226	1.00	79.39	B
ATOM	144	CA	LYS	34	63.853	1.029	55.284	1.00	80.19	B
ATOM	145	CB	LYS	34	63.984	2.543	55.504	1.00	81.11	B
ATOM	146	CG	LYS	34	64.392	3.347	54.267	1.00	82.59	B
ATOM	147	CD	LYS	34	65.910	3.501	54.147	1.00	83.41	B
ATOM	148	CE	LYS	34	66.604	2.186	53.810	1.00	84.19	B
ATOM	149	NZ	LYS	34	68.089	2.305	53.845	1.00	84.38	B
ATOM	150	C	LYS	34	64.539	0.285	56.423	1.00	80.45	B
ATOM	151	O	LYS	34	65.757	0.159	56.448	1.00	81.20	B
ATOM	152	N	ALA	35	63.740	-0.209	57.365	1.00	80.19	B
ATOM	153	CA	ALA	35	64.264	-0.946	58.509	1.00	79.99	B
ATOM	154	CB	ALA	35	63.654	-0.405	59.800	1.00	79.19	B
ATOM	155	C	ALA	35	63.966	-2.441	58.372	1.00	79.54	B
ATOM	156	O	ALA	35	64.029	-3.181	59.347	1.00	79.52	B
ATOM	157	N	SER	36	63.650	-2.870	57.150	1.00	79.23	B
ATOM	158	CA	SER	36	63.324	-4.269	56.866	1.00	78.90	B
ATOM	159	CB	SER	36	64.581	-5.140	56.934	1.00	79.55	B
ATOM	160	OG	SER	36	65.497	-4.786	55.913	1.00	80.94	B
ATOM	161	C	SER	36	62.291	-4.773	57.863	1.00	77.94	B
ATOM	162	O	SER	36	62.621	-5.460	58.826	1.00	78.06	B
ATOM	163	N	ALA	37	61.033	-4.422	57.620	1.00	76.14	B
ATOM	164	CA	ALA	37	59.952	-4.822	58.505	1.00	74.02	B
ATOM	165	CB	ALA	37	58.862	-3.763	58.496	1.00	74.76	B
ATOM	166	C	ALA	37	59.370	-6.177	58.128	1.00	72.27	B
ATOM	167	O	ALA	37	59.282	-6.526	56.956	1.00	71.83	B
ATOM	168	N	HIS	38	58.975	-6.928	59.151	1.00	70.33	B
ATOM	169	CA	HIS	38	58.388	-8.249	58.981	1.00	67.10	B
ATOM	170	CB	HIS	38	59.039	-9.236	59.961	1.00	69.95	B
ATOM	171	CG	HIS	38	59.177	-8.706	61.358	1.00	72.03	B
ATOM	172	CD2	HIS	38	58.589	-9.085	62.518	1.00	72.68	B
ATOM	173	ND1	HIS	38	60.004	-7.648	61.676	1.00	72.05	B
ATOM	174	CE1	HIS	38	59.919	-7.399	62.971	1.00	72.38	B
ATOM	175	NE2	HIS	38	59.067	-8.256	63.505	1.00	73.14	B
ATOM	176	C	HIS	38	56.877	-8.187	59.220	1.00	63.55	B
ATOM	177	O	HIS	38	56.426	-7.917	60.335	1.00	63.33	B
ATOM	178	N	SER	39	56.100	-8.432	58.168	1.00	58.67	B
ATOM	179	CA	SER	39	54.643	-8.399	58.266	1.00	54.45	B
ATOM	180	CB	SER	39	54.005	-8.478	56.879	1.00	53.84	B
ATOM	181	OG	SER	39	52.595	-8.614	56.976	1.00	49.31	B
ATOM	182	C	SER	39	54.081	-9.519	59.122	1.00	52.25	B
ATOM	183	O	SER	39	54.384	-10.686	58.910	1.00	51.84	B
ATOM	184	N	ILE	40	53.251	-9.149	60.089	1.00	49.22	B
ATOM	185	CA	ILE	40	52.631	-10.122	60.967	1.00	47.52	B
ATOM	186	CB	ILE	40	52.679	-9.674	62.444	1.00	45.91	B
ATOM	187	CG2	ILE	40	54.115	-9.499	62.881	1.00	44.82	B
ATOM	188	CG1	ILE	40	51.915	-8.361	62.622	1.00	45.54	B
ATOM	189	CD1	ILE	40	51.580	-8.050	64.066	1.00	46.62	B
ATOM	190	C	ILE	40	51.176	-10.316	60.557	1.00	47.28	B
ATOM	191	O	ILE	40	50.421	-10.994	61.234	1.00	46.90	B
ATOM	192	N	VAL	41	50.798	-9.718	59.433	1.00	47.41	B
ATOM	193	CA	VAL	41	49.430	-9.824	58.939	1.00	48.95	B
ATOM	194	CB	VAL	41	48.713	-8.450	58.983	1.00	49.16	B
ATOM	195	CG1	VAL	41	47.290	-8.585	58.467	1.00	49.01	B
ATOM	196	CG2	VAL	41	48.713	-7.903	60.402	1.00	49.06	B
ATOM	197	C	VAL	41	49.395	-10.347	57.509	1.00	49.67	B
ATOM	198	O	VAL	41	50.004	-9.777	56.620	1.00	49.95	B
ATOM	199	N	GLU	42	48.685	-11.449	57.301	1.00	50.48	B
ATOM	200	CA	GLU	42	48.575	-12.024	55.969	1.00	51.59	B
ATOM	201	CB	GLU	42	49.176	-13.434	55.935	1.00	52.66	B
ATOM	202	CG	GLU	42	50.609	-13.510	56.447	1.00	56.16	B
ATOM	203	CD	GLU	42	51.164	-14.931	56.476	1.00	58.24	B
ATOM	204	OE1	GLU	42	50.430	-15.854	56.899	1.00	57.80	B
ATOM	205	OE2	GLU	42	52.338	-15.119	56.081	1.00	58.28	B
ATOM	206	C	GLU	42	47.102	-12.072	55.599	1.00	50.83	B
ATOM	207	O	GLU	42	46.283	-12.604	56.343	1.00	51.55	B
ATOM	208	N	CYS	43	46.768	-11.493	54.453	1.00	49.80	B
ATOM	209	CA	CYS	43	45.389	-11.473	53.995	1.00	49.65	B
ATOM	210	CB	CYS	43	45.037	-10.087	53.433	1.00	49.93	B

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ATOM    211  SG  CYS    43      45.019  -8.745  54.661  1.00 48.78      B
ATOM    212  C   CYS    43      45.140 -12.535  52.931  1.00 48.94      B
ATOM    213  O   CYS    43      46.010 -12.833  52.123  1.00 48.97      B
ATOM    214  N   ASP    44      43.939 -13.105  52.954  1.00 49.14      B
ATOM    215  CA  ASP    44      43.534 -14.121  51.992  1.00 48.86      B
ATOM    216  CB  ASP    44      43.463 -15.494  52.660  1.00 50.97      B
ATOM    217  CG  ASP    44      43.589 -16.635  51.666  1.00 52.32      B
ATOM    218  OD1 ASP    44      43.126 -16.483  50.510  1.00 52.22      B
ATOM    219  OD2 ASP    44      44.147 -17.689  52.048  1.00 52.81      B
ATOM    220  C   ASP    44      42.150 -13.749  51.456  1.00 48.60      B
ATOM    221  O   ASP    44      41.127 -14.147  52.012  1.00 46.42      B
ATOM    222  N   PRO    45      42.108 -12.969  50.364  1.00 48.35      B
ATOM    223  CD  PRO    45      43.252 -12.517  49.557  1.00 48.19      B
ATOM    224  CA  PRO    45      40.847 -12.540  49.755  1.00 48.75      B
ATOM    225  CB  PRO    45      41.307 -11.680  48.584  1.00 49.00      B
ATOM    226  CG  PRO    45      42.617 -12.306  48.211  1.00 49.04      B
ATOM    227  C   PRO    45      39.957 -13.688  49.312  1.00 50.08      B
ATOM    228  O   PRO    45      38.750 -13.661  49.535  1.00 50.55      B
ATOM    229  N   VAL    46      40.561 -14.693  48.683  1.00 50.66      B
ATOM    230  CA  VAL    46      39.818 -15.851  48.213  1.00 50.49      B
ATOM    231  CB  VAL    46      40.745 -16.853  47.500  1.00 50.30      B
ATOM    232  CG1 VAL    46      39.957 -18.079  47.077  1.00 49.67      B
ATOM    233  CG2 VAL    46      41.393 -16.192  46.293  1.00 49.30      B
ATOM    234  C   VAL    46      39.145 -16.545  49.389  1.00 50.88      B
ATOM    235  O   VAL    46      37.965 -16.870  49.338  1.00 52.16      B
ATOM    236  N   ARG    47      39.906 -16.761  50.454  1.00 49.91      B
ATOM    237  CA  ARG    47      39.369 -17.417  51.635  1.00 49.25      B
ATOM    238  CB  ARG    47      40.499 -18.074  52.431  1.00 53.01      B
ATOM    239  CG  ARG    47      40.025 -19.009  53.535  1.00 58.79      B
ATOM    240  CD  ARG    47      39.711 -20.404  52.993  1.00 62.76      B
ATOM    241  NE  ARG    47      40.925 -21.094  52.566  1.00 65.61      B
ATOM    242  CZ  ARG    47      41.887 -21.489  53.395  1.00 67.31      B
ATOM    243  NH1 ARG    47      41.770 -21.265  54.699  1.00 67.77      B
ATOM    244  NH2 ARG    47      42.970 -22.093  52.922  1.00 67.97      B
ATOM    245  C   ARG    47      38.649 -16.396  52.518  1.00 46.27      B
ATOM    246  O   ARG    47      37.980 -16.767  53.479  1.00 45.17      B
ATOM    247  N   LYS    48      38.789 -15.116  52.167  1.00 43.30      B
ATOM    248  CA  LYS    48      38.191 -14.003  52.911  1.00 40.30      B
ATOM    249  CB  LYS    48      36.660 -14.063  52.861  1.00 40.48      B
ATOM    250  CG  LYS    48      36.074 -13.999  51.466  1.00 42.10      B
ATOM    251  CD  LYS    48      34.566 -14.224  51.491  1.00 46.49      B
ATOM    252  CE  LYS    48      34.011 -14.463  50.088  1.00 48.94      B
ATOM    253  NZ  LYS    48      34.342 -13.358  49.137  1.00 51.33      B
ATOM    254  C   LYS    48      38.649 -14.040  54.364  1.00 38.40      B
ATOM    255  O   LYS    48      37.879 -13.780  55.271  1.00 37.06      B
ATOM    256  N   GLU    49      39.918 -14.374  54.573  1.00 38.43      B
ATOM    257  CA  GLU    49      40.472 -14.451  55.918  1.00 38.68      B
ATOM    258  CB  GLU    49      40.965 -15.867  56.237  1.00 42.04      B
ATOM    259  CG  GLU    49      39.896 -16.940  56.342  1.00 47.74      B
ATOM    260  CD  GLU    49      40.478 -18.320  56.671  1.00 49.86      B
ATOM    261  OE1 GLU    49      39.706 -19.305  56.666  1.00 50.42      B
ATOM    262  OE2 GLU    49      41.701 -18.419  56.930  1.00 49.85      B
ATOM    263  C   GLU    49      41.643 -13.506  56.111  1.00 37.41      B
ATOM    264  O   GLU    49      42.273 -13.066  55.158  1.00 34.84      B
ATOM    265  N   VAL    50      41.925 -13.220  57.374  1.00 36.48      B
ATOM    266  CA  VAL    50      43.035 -12.366  57.751  1.00 37.37      B
ATOM    267  CB  VAL    50      42.539 -10.930  58.146  1.00 37.30      B
ATOM    268  CG1 VAL    50      41.332 -11.008  59.061  1.00 38.02      B
ATOM    269  CG2 VAL    50      43.655 -10.153  58.813  1.00 36.20      B
ATOM    270  C   VAL    50      43.709 -13.074  58.921  1.00 36.84      B
ATOM    271  O   VAL    50      43.078 -13.354  59.926  1.00 37.07      B
ATOM    272  N   SER    51      44.988 -13.399  58.772  1.00 37.03      B
ATOM    273  CA  SER    51      45.702 -14.095  59.835  1.00 37.03      B
ATOM    274  CB  SER    51      46.315 -15.390  59.294  1.00 37.38      B
ATOM    275  OG  SER    51      46.507 -16.327  60.339  1.00 38.42      B
ATOM    276  C   SER    51      46.791 -13.217  60.436  1.00 37.30      B
ATOM    277  O   SER    51      47.538 -12.567  59.712  1.00 37.32      B
ATOM    278  N   VAL    52      46.870 -13.207  61.764  1.00 37.43      B
ATOM    279  CA  VAL    52      47.861 -12.398  62.476  1.00 40.09      B
ATOM    280  CB  VAL    52      47.170 -11.380  63.433  1.00 38.82      B
ATOM    281  CG1 VAL    52      48.210 -10.529  64.140  1.00 38.44      B
ATOM    282  CG2 VAL    52      46.207 -10.507  62.664  1.00 39.75      B
ATOM    283  C   VAL    52      48.814 -13.254  63.307  1.00 41.41      B
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ATOM	284	O	VAL	52	48.383	-14.120	64.059	1.00	42.26	B
ATOM	285	N	ARG	53	50.112	-13.001	63.170	1.00	42.93	B
ATOM	286	CA	ARG	53	51.115	-13.746	63.922	1.00	44.63	B
ATOM	287	CB	ARG	53	52.435	-13.782	63.156	1.00	44.21	B
ATOM	288	CG	ARG	53	53.621	-14.258	63.976	1.00	45.18	B
ATOM	289	CD	ARG	53	54.721	-14.772	63.069	1.00	47.32	B
ATOM	290	NE	ARG	53	55.045	-13.815	62.016	1.00	48.93	B
ATOM	291	CZ	ARG	53	55.538	-14.154	60.831	1.00	48.81	B
ATOM	292	NH1	ARG	53	55.762	-15.430	60.548	1.00	49.29	B
ATOM	293	NH2	ARG	53	55.804	-13.221	59.928	1.00	50.89	B
ATOM	294	C	ARG	53	51.333	-13.130	65.298	1.00	46.43	B
ATOM	295	O	ARG	53	51.867	-12.030	65.420	1.00	47.02	B
ATOM	296	N	THR	54	50.915	-13.855	66.331	1.00	48.25	B
ATOM	297	CA	THR	54	51.052	-13.401	67.711	1.00	50.92	B
ATOM	298	CB	THR	54	49.768	-13.683	68.512	1.00	50.31	B
ATOM	299	OG1	THR	54	49.572	-15.098	68.631	1.00	50.23	B
ATOM	300	CG2	THR	54	48.567	-13.078	67.810	1.00	50.24	B
ATOM	301	C	THR	54	52.211	-14.097	68.412	1.00	53.34	B
ATOM	302	O	THR	54	52.551	-13.769	69.538	1.00	53.13	B
ATOM	303	N	GLY	55	52.815	-15.059	67.726	1.00	57.17	B
ATOM	304	CA	GLY	55	53.917	-15.805	68.303	1.00	61.42	B
ATOM	305	C	GLY	55	55.300	-15.366	67.868	1.00	64.33	B
ATOM	306	O	GLY	55	55.566	-14.175	67.715	1.00	65.05	B
ATOM	307	N	GLY	56	56.181	-16.346	67.672	1.00	66.22	B
ATOM	308	CA	GLY	56	57.548	-16.061	67.272	1.00	68.09	B
ATOM	309	C	GLY	56	57.760	-15.914	65.777	1.00	69.96	B
ATOM	310	O	GLY	56	56.950	-15.305	65.084	1.00	70.41	B
ATOM	311	N	LEU	57	58.860	-16.484	65.288	1.00	71.01	B
ATOM	312	CA	LEU	57	59.220	-16.421	63.873	1.00	70.64	B
ATOM	313	CB	LEU	57	60.702	-16.771	63.704	1.00	71.42	B
ATOM	314	CG	LEU	57	61.326	-17.671	64.778	1.00	71.92	B
ATOM	315	CD1	LEU	57	60.653	-19.034	64.777	1.00	72.30	B
ATOM	316	CD2	LEU	57	62.819	-17.813	64.522	1.00	72.27	B
ATOM	317	C	LEU	57	58.366	-17.311	62.973	1.00	70.34	B
ATOM	318	O	LEU	57	57.535	-18.083	63.450	1.00	69.85	B
ATOM	319	N	ALA	58	58.589	-17.189	61.667	1.00	69.38	B
ATOM	320	CA	ALA	58	57.852	-17.959	60.669	1.00	68.14	B
ATOM	321	CB	ALA	58	58.169	-17.430	59.268	1.00	68.25	B
ATOM	322	C	ALA	58	58.129	-19.462	60.742	1.00	66.52	B
ATOM	323	O	ALA	58	57.262	-20.268	60.433	1.00	66.64	B
ATOM	324	N	ASP	59	59.343	-19.825	61.150	1.00	64.49	B
ATOM	325	CA	ASP	59	59.743	-21.226	61.270	1.00	62.67	B
ATOM	326	CB	ASP	59	61.183	-21.310	61.798	1.00	62.19	B
ATOM	327	CG	ASP	59	61.589	-22.724	62.197	1.00	61.33	B
ATOM	328	OD1	ASP	59	61.727	-23.594	61.307	1.00	59.84	B
ATOM	329	OD2	ASP	59	61.772	-22.963	63.410	1.00	60.73	B
ATOM	330	C	ASP	59	58.801	-21.994	62.201	1.00	61.33	B
ATOM	331	O	ASP	59	58.542	-23.182	62.005	1.00	60.81	B
ATOM	332	N	LYS	60	58.287	-21.302	63.211	1.00	59.03	B
ATOM	333	CA	LYS	60	57.376	-21.897	64.179	1.00	57.28	B
ATOM	334	CB	LYS	60	58.147	-22.816	65.134	1.00	57.38	B
ATOM	335	CG	LYS	60	57.281	-23.524	66.164	1.00	57.92	B
ATOM	336	CD	LYS	60	58.117	-24.299	67.172	1.00	58.61	B
ATOM	337	CE	LYS	60	57.247	-24.930	68.245	1.00	58.86	B
ATOM	338	NZ	LYS	60	58.064	-25.535	69.333	1.00	59.92	B
ATOM	339	C	LYS	60	56.710	-20.771	64.968	1.00	55.75	B
ATOM	340	O	LYS	60	57.391	-19.942	65.574	1.00	55.85	B
ATOM	341	N	SER	61	55.381	-20.735	64.953	1.00	52.88	B
ATOM	342	CA	SER	61	54.655	-19.692	65.666	1.00	50.87	B
ATOM	343	CB	SER	61	54.863	-18.343	64.967	1.00	50.80	B
ATOM	344	OG	SER	61	54.294	-18.346	63.667	1.00	48.16	B
ATOM	345	C	SER	61	53.158	-19.957	65.796	1.00	50.20	B
ATOM	346	O	SER	61	52.630	-20.909	65.245	1.00	49.59	B
ATOM	347	N	SER	62	52.493	-19.086	66.547	1.00	49.11	B
ATOM	348	CA	SER	62	51.055	-19.170	66.752	1.00	48.21	B
ATOM	349	CB	SER	62	50.732	-19.101	68.248	1.00	48.08	B
ATOM	350	OG	SER	62	51.371	-17.993	68.858	1.00	48.30	B
ATOM	351	C	SER	62	50.421	-17.990	66.010	1.00	48.13	B
ATOM	352	O	SER	62	51.097	-17.016	65.703	1.00	47.13	B
ATOM	353	N	ARG	63	49.129	-18.085	65.712	1.00	47.13	B
ATOM	354	CA	ARG	63	48.441	-17.015	64.998	1.00	45.05	B
ATOM	355	CB	ARG	63	48.539	-17.231	63.481	1.00	44.51	B
ATOM	356	CG	ARG	63	49.960	-17.194	62.925	1.00	44.98	B

ATOM	357	CD	ARG	63	49.976	-17.466	61.428	1.00	46.63	B
ATOM	358	NE	ARG	63	49.443	-16.349	60.645	1.00	48.69	B
ATOM	359	CZ	ARG	63	50.148	-15.285	60.263	1.00	48.66	B
ATOM	360	NH1	ARG	63	51.429	-15.178	60.587	1.00	49.48	B
ATOM	361	NH2	ARG	63	49.574	-14.329	59.545	1.00	48.53	B
ATOM	362	C	ARG	63	46.975	-16.918	65.401	1.00	43.84	B
ATOM	363	O	ARG	63	46.477	-17.726	66.176	1.00	44.06	B
ATOM	364	N	LYS	64	46.305	-15.902	64.868	1.00	42.24	B
ATOM	365	CA	LYS	64	44.892	-15.652	65.124	1.00	40.40	B
ATOM	366	CB	LYS	64	44.723	-14.434	66.032	1.00	41.92	B
ATOM	367	CG	LYS	64	45.181	-14.635	67.470	1.00	43.37	B
ATOM	368	CD	LYS	64	44.088	-15.261	68.317	1.00	43.81	B
ATOM	369	CE	LYS	64	44.446	-15.213	69.794	1.00	45.77	B
ATOM	370	NZ	LYS	64	43.374	-15.792	70.658	1.00	46.88	B
ATOM	371	C	LYS	64	44.257	-15.369	63.771	1.00	39.22	B
ATOM	372	O	LYS	64	44.631	-14.405	63.102	1.00	39.99	B
ATOM	373	N	THR	65	43.312	-16.210	63.361	1.00	36.46	B
ATOM	374	CA	THR	65	42.656	-16.031	62.074	1.00	34.76	B
ATOM	375	CB	THR	65	42.745	-17.323	61.212	1.00	35.41	B
ATOM	376	OG1	THR	65	44.118	-17.692	61.041	1.00	32.86	B
ATOM	377	CG2	THR	65	42.130	-17.090	59.826	1.00	36.73	B
ATOM	378	C	THR	65	41.194	-15.638	62.238	1.00	34.16	B
ATOM	379	O	THR	65	40.477	-16.200	63.070	1.00	35.43	B
ATOM	380	N	TYR	66	40.764	-14.660	61.448	1.00	30.66	B
ATOM	381	CA	TYR	66	39.391	-14.181	61.488	1.00	28.38	B
ATOM	382	CB	TYR	66	39.337	-12.765	62.072	1.00	25.32	B
ATOM	383	CG	TYR	66	39.886	-12.652	63.473	1.00	22.38	B
ATOM	384	CD1	TYR	66	41.255	-12.566	63.710	1.00	20.36	B
ATOM	385	CE1	TYR	66	41.753	-12.475	65.011	1.00	19.50	B
ATOM	386	CD2	TYR	66	39.027	-12.647	64.569	1.00	22.45	B
ATOM	387	CE2	TYR	66	39.506	-12.559	65.868	1.00	19.18	B
ATOM	388	CZ	TYR	66	40.865	-12.470	66.086	1.00	21.06	B
ATOM	389	OH	TYR	66	41.317	-12.358	67.391	1.00	25.17	B
ATOM	390	C	TYR	66	38.815	-14.171	60.076	1.00	29.18	B
ATOM	391	O	TYR	66	39.537	-13.953	59.108	1.00	29.59	B
ATOM	392	N	THR	67	37.514	-14.418	59.963	1.00	30.96	B
ATOM	393	CA	THR	67	36.854	-14.420	58.662	1.00	31.82	B
ATOM	394	CB	THR	67	36.083	-15.742	58.418	1.00	31.49	B
ATOM	395	OG1	THR	67	36.983	-16.849	58.543	1.00	35.18	B
ATOM	396	CG2	THR	67	35.482	-15.759	57.016	1.00	30.30	B
ATOM	397	C	THR	67	35.873	-13.252	58.565	1.00	31.85	B
ATOM	398	O	THR	67	35.100	-12.996	59.504	1.00	32.04	B
ATOM	399	N	PHE	68	35.923	-12.536	57.442	1.00	29.70	B
ATOM	400	CA	PHE	68	35.029	-11.400	57.203	1.00	31.18	B
ATOM	401	CB	PHE	68	35.785	-10.063	57.305	1.00	29.26	B
ATOM	402	CG	PHE	68	36.374	-9.797	58.658	1.00	27.25	B
ATOM	403	CD1	PHE	68	37.617	-10.309	59.001	1.00	28.36	B
ATOM	404	CD2	PHE	68	35.666	-9.071	59.611	1.00	28.98	B
ATOM	405	CE1	PHE	68	38.147	-10.110	60.277	1.00	27.66	B
ATOM	406	CE2	PHE	68	36.188	-8.867	60.894	1.00	27.30	B
ATOM	407	CZ	PHE	68	37.430	-9.388	61.225	1.00	26.68	B
ATOM	408	C	PHE	68	34.418	-11.527	55.815	1.00	30.88	B
ATOM	409	O	PHE	68	34.814	-12.385	55.032	1.00	32.33	B
ATOM	410	N	ASP	69	33.452	-10.670	55.514	1.00	30.45	B
ATOM	411	CA	ASP	69	32.796	-10.702	54.212	1.00	31.77	B
ATOM	412	CB	ASP	69	31.636	-9.698	54.185	1.00	33.60	B
ATOM	413	CG	ASP	69	30.590	-9.988	55.258	1.00	36.34	B
ATOM	414	OD1	ASP	69	30.514	-9.221	56.254	1.00	35.89	B
ATOM	415	OD2	ASP	69	29.856	-10.995	55.112	1.00	33.96	B
ATOM	416	C	ASP	69	33.775	-10.414	53.078	1.00	30.67	B
ATOM	417	O	ASP	69	33.594	-10.882	51.970	1.00	31.26	B
ATOM	418	N	MET	70	34.816	-9.646	53.377	1.00	31.20	B
ATOM	419	CA	MET	70	35.836	-9.294	52.394	1.00	31.00	B
ATOM	420	CB	MET	70	35.396	-8.081	51.567	1.00	33.24	B
ATOM	421	CG	MET	70	34.253	-8.330	50.598	1.00	35.15	B
ATOM	422	SD	MET	70	33.994	-6.921	49.476	1.00	43.03	B
ATOM	423	CE	MET	70	32.288	-6.531	49.777	1.00	42.27	B
ATOM	424	C	MET	70	37.158	-8.978	53.090	1.00	29.72	B
ATOM	425	O	MET	70	37.186	-8.682	54.271	1.00	29.23	B
ATOM	426	N	VAL	71	38.257	-9.052	52.353	1.00	28.80	B
ATOM	427	CA	VAL	71	39.561	-8.765	52.929	1.00	30.15	B
ATOM	428	CB	VAL	71	40.256	-10.054	53.443	1.00	31.84	B
ATOM	429	CG1	VAL	71	41.603	-9.713	54.060	1.00	33.61	B

ATOM	430	CG2	VAL	71	39.388	-10.738	54.471	1.00	31.83	B
ATOM	431	C	VAL	71	40.439	-8.102	51.878	1.00	29.25	B
ATOM	432	O	VAL	71	40.471	-8.526	50.734	1.00	30.25	B
ATOM	433	N	PHE	72	41.146	-7.053	52.285	1.00	30.15	B
ATOM	434	CA	PHE	72	42.015	-6.306	51.384	1.00	30.67	B
ATOM	435	CB	PHE	72	41.445	-4.905	51.152	1.00	28.16	B
ATOM	436	CG	PHE	72	40.060	-4.903	50.573	1.00	27.42	B
ATOM	437	CD1	PHE	72	39.854	-5.145	49.220	1.00	26.23	B
ATOM	438	CD2	PHE	72	38.955	-4.686	51.390	1.00	26.64	B
ATOM	439	CE1	PHE	72	38.565	-5.171	48.688	1.00	25.66	B
ATOM	440	CE2	PHE	72	37.664	-4.709	50.868	1.00	25.86	B
ATOM	441	CZ	PHE	72	37.469	-4.954	49.516	1.00	24.73	B
ATOM	442	C	PHE	72	43.428	-6.188	51.940	1.00	31.84	B
ATOM	443	O	PHE	72	43.646	-5.560	52.973	1.00	30.82	B
ATOM	444	N	GLY	73	44.385	-6.797	51.247	1.00	32.27	B
ATOM	445	CA	GLY	73	45.757	-6.727	51.697	1.00	32.67	B
ATOM	446	C	GLY	73	46.358	-5.377	51.366	1.00	33.72	B
ATOM	447	O	GLY	73	45.730	-4.553	50.707	1.00	33.21	B
ATOM	448	N	ALA	74	47.589	-5.163	51.815	1.00	34.20	B
ATOM	449	CA	ALA	74	48.296	-3.911	51.583	1.00	35.80	B
ATOM	450	CB	ALA	74	49.615	-3.929	52.329	1.00	35.10	B
ATOM	451	C	ALA	74	48.547	-3.664	50.100	1.00	37.02	B
ATOM	452	O	ALA	74	49.235	-2.734	49.730	1.00	38.45	B
ATOM	453	N	SER	75	47.971	-4.498	49.250	1.00	38.40	B
ATOM	454	CA	SER	75	48.179	-4.356	47.821	1.00	40.23	B
ATOM	455	CB	SER	75	48.437	-5.733	47.204	1.00	40.06	B
ATOM	456	OG	SER	75	47.371	-6.617	47.504	1.00	38.50	B
ATOM	457	C	SER	75	46.990	-3.701	47.126	1.00	40.71	B
ATOM	458	O	SER	75	47.155	-3.026	46.109	1.00	40.44	B
ATOM	459	N	THR	76	45.795	-3.917	47.677	1.00	40.56	B
ATOM	460	CA	THR	76	44.568	-3.365	47.107	1.00	40.11	B
ATOM	461	CB	THR	76	43.325	-3.769	47.960	1.00	41.15	B
ATOM	462	OG1	THR	76	43.690	-3.865	49.342	1.00	43.22	B
ATOM	463	CG2	THR	76	42.774	-5.118	47.498	1.00	43.01	B
ATOM	464	C	THR	76	44.615	-1.849	46.937	1.00	38.50	B
ATOM	465	O	THR	76	45.071	-1.119	47.819	1.00	38.53	B
ATOM	466	N	LYS	77	44.152	-1.385	45.785	1.00	36.21	B
ATOM	467	CA	LYS	77	44.135	0.036	45.483	1.00	34.26	B
ATOM	468	CB	LYS	77	44.482	0.243	44.011	1.00	36.10	B
ATOM	469	CG	LYS	77	45.901	-0.174	43.651	1.00	39.66	B
ATOM	470	CD	LYS	77	46.138	-0.013	42.153	1.00	43.10	B
ATOM	471	CE	LYS	77	47.538	-0.446	41.749	1.00	44.09	B
ATOM	472	NZ	LYS	77	47.693	-0.451	40.261	1.00	46.93	B
ATOM	473	C	LYS	77	42.776	0.662	45.799	1.00	32.74	B
ATOM	474	O	LYS	77	41.807	-0.045	46.049	1.00	30.61	B
ATOM	475	N	GLN	78	42.729	1.994	45.800	1.00	31.08	B
ATOM	476	CA	GLN	78	41.499	2.731	46.084	1.00	29.81	B
ATOM	477	CB	GLN	78	41.718	4.241	45.896	1.00	29.96	B
ATOM	478	CG	GLN	78	42.791	4.867	46.790	1.00	28.93	B
ATOM	479	CD	GLN	78	42.339	5.029	48.224	1.00	28.69	B
ATOM	480	OE1	GLN	78	41.731	4.136	48.789	1.00	28.17	B
ATOM	481	NE2	GLN	78	42.647	6.177	48.822	1.00	28.63	B
ATOM	482	C	GLN	78	40.371	2.273	45.160	1.00	29.13	B
ATOM	483	O	GLN	78	39.255	2.045	45.597	1.00	28.04	B
ATOM	484	N	ILE	79	40.687	2.140	43.877	1.00	27.65	B
ATOM	485	CA	ILE	79	39.710	1.730	42.874	1.00	28.90	B
ATOM	486	CB	ILE	79	40.369	1.664	41.472	1.00	28.34	B
ATOM	487	CG2	ILE	79	41.411	0.564	41.442	1.00	30.45	B
ATOM	488	CG1	ILE	79	39.316	1.396	40.400	1.00	29.43	B
ATOM	489	CD1	ILE	79	38.333	2.517	40.226	1.00	30.66	B
ATOM	490	C	ILE	79	39.055	0.377	43.191	1.00	28.47	B
ATOM	491	O	ILE	79	37.867	0.175	42.938	1.00	27.79	B
ATOM	492	N	ASP	80	39.829	-0.548	43.749	1.00	28.15	B
ATOM	493	CA	ASP	80	39.296	-1.866	44.076	1.00	27.60	B
ATOM	494	CB	ASP	80	40.435	-2.865	44.316	1.00	27.34	B
ATOM	495	CG	ASP	80	41.439	-2.908	43.164	1.00	29.59	B
ATOM	496	OD1	ASP	80	41.018	-2.784	41.987	1.00	27.17	B
ATOM	497	OD2	ASP	80	42.648	-3.078	43.445	1.00	29.79	B
ATOM	498	C	ASP	80	38.395	-1.800	45.303	1.00	27.71	B
ATOM	499	O	ASP	80	37.394	-2.492	45.383	1.00	27.27	B
ATOM	500	N	VAL	81	38.761	-0.964	46.265	1.00	28.05	B
ATOM	501	CA	VAL	81	37.947	-0.820	47.460	1.00	27.29	B
ATOM	502	CB	VAL	81	38.618	0.115	48.495	1.00	25.22	B

ATOM	503	CG1	VAL	81	37.662	0.394	49.633	1.00	21.33	B
ATOM	504	CG2	VAL	81	39.890	-0.532	49.036	1.00	23.97	B
ATOM	505	C	VAL	81	36.588	-0.244	47.079	1.00	28.97	B
ATOM	506	O	VAL	81	35.555	-0.682	47.590	1.00	29.68	B
ATOM	507	N	TYR	82	36.593	0.721	46.162	1.00	28.62	B
ATOM	508	CA	TYR	82	35.364	1.368	45.723	1.00	30.02	B
ATOM	509	CB	TYR	82	35.693	2.640	44.924	1.00	31.49	B
ATOM	510	CG	TYR	82	34.472	3.389	44.443	1.00	33.00	B
ATOM	511	CD1	TYR	82	33.934	3.144	43.180	1.00	34.00	B
ATOM	512	CE1	TYR	82	32.776	3.781	42.762	1.00	37.72	B
ATOM	513	CD2	TYR	82	33.817	4.299	45.278	1.00	32.60	B
ATOM	514	CE2	TYR	82	32.659	4.938	44.871	1.00	36.04	B
ATOM	515	CZ	TYR	82	32.142	4.676	43.613	1.00	39.42	B
ATOM	516	OH	TYR	82	30.992	5.316	43.203	1.00	42.75	B
ATOM	517	C	TYR	82	34.456	0.451	44.906	1.00	30.88	B
ATOM	518	O	TYR	82	33.264	0.363	45.168	1.00	30.76	B
ATOM	519	N	ARG	83	35.021	-0.223	43.910	1.00	32.85	B
ATOM	520	CA	ARG	83	34.239	-1.136	43.077	1.00	34.09	B
ATOM	521	CB	ARG	83	35.120	-1.702	41.965	1.00	35.60	B
ATOM	522	CG	ARG	83	35.333	-0.749	40.798	1.00	42.48	B
ATOM	523	CD	ARG	83	36.652	-1.013	40.072	1.00	46.99	B
ATOM	524	NE	ARG	83	36.734	-2.358	39.503	1.00	53.06	B
ATOM	525	CZ	ARG	83	36.100	-2.758	38.404	1.00	56.78	B
ATOM	526	NH1	ARG	83	35.323	-1.914	37.735	1.00	57.61	B
ATOM	527	NH2	ARG	83	36.254	-4.004	37.967	1.00	57.03	B
ATOM	528	C	ARG	83	33.630	-2.277	43.895	1.00	33.36	B
ATOM	529	O	ARG	83	32.492	-2.674	43.667	1.00	34.00	B
ATOM	530	N	SER	84	34.390	-2.785	44.860	1.00	31.69	B
ATOM	531	CA	SER	84	33.956	-3.899	45.701	1.00	30.91	B
ATOM	532	CB	SER	84	35.180	-4.582	46.322	1.00	31.88	B
ATOM	533	OG	SER	84	36.115	-4.951	45.324	1.00	34.36	B
ATOM	534	C	SER	84	32.983	-3.535	46.816	1.00	30.39	B
ATOM	535	O	SER	84	31.963	-4.195	47.007	1.00	30.60	B
ATOM	536	N	VAL	85	33.299	-2.489	47.568	1.00	29.66	B
ATOM	537	CA	VAL	85	32.432	-2.091	48.663	1.00	28.01	B
ATOM	538	CB	VAL	85	33.255	-1.652	49.887	1.00	27.01	B
ATOM	539	CG1	VAL	85	32.336	-1.128	50.971	1.00	26.26	B
ATOM	540	CG2	VAL	85	34.080	-2.815	50.407	1.00	26.27	B
ATOM	541	C	VAL	85	31.445	-0.983	48.337	1.00	27.47	B
ATOM	542	O	VAL	85	30.249	-1.149	48.498	1.00	28.23	B
ATOM	543	N	VAL	86	31.960	0.145	47.868	1.00	28.02	B
ATOM	544	CA	VAL	86	31.132	1.313	47.585	1.00	28.51	B
ATOM	545	CB	VAL	86	32.004	2.568	47.370	1.00	26.65	B
ATOM	546	CG1	VAL	86	31.180	3.808	47.625	1.00	25.89	B
ATOM	547	CG2	VAL	86	33.220	2.532	48.267	1.00	25.41	B
ATOM	548	C	VAL	86	30.150	1.224	46.425	1.00	29.30	B
ATOM	549	O	VAL	86	28.959	1.479	46.599	1.00	28.44	B
ATOM	550	N	CYS	87	30.649	0.881	45.244	1.00	29.85	B
ATOM	551	CA	CYS	87	29.802	0.786	44.064	1.00	33.34	B
ATOM	552	CB	CYS	87	30.549	0.025	42.965	1.00	36.49	B
ATOM	553	SG	CYS	87	29.936	0.313	41.286	1.00	43.07	B
ATOM	554	C	CYS	87	28.445	0.131	44.373	1.00	34.93	B
ATOM	555	O	CYS	87	27.396	0.670	44.026	1.00	34.18	B
ATOM	556	N	PRO	88	28.452	-1.035	45.045	1.00	35.57	B
ATOM	557	CD	PRO	88	29.603	-1.876	45.420	1.00	37.48	B
ATOM	558	CA	PRO	88	27.195	-1.715	45.378	1.00	35.50	B
ATOM	559	CB	PRO	88	27.664	-2.989	46.078	1.00	35.52	B
ATOM	560	CG	PRO	88	28.984	-3.247	45.464	1.00	36.85	B
ATOM	561	C	PRO	88	26.295	-0.874	46.287	1.00	35.13	B
ATOM	562	O	PRO	88	25.099	-0.765	46.050	1.00	35.74	B
ATOM	563	N	ILE	89	26.885	-0.288	47.327	1.00	34.00	B
ATOM	564	CA	ILE	89	26.140	0.535	48.279	1.00	33.52	B
ATOM	565	CB	ILE	89	27.031	0.978	49.465	1.00	33.84	B
ATOM	566	CG2	ILE	89	26.250	1.910	50.384	1.00	34.73	B
ATOM	567	CG1	ILE	89	27.514	-0.247	50.243	1.00	33.35	B
ATOM	568	CD1	ILE	89	28.486	0.077	51.357	1.00	33.52	B
ATOM	569	C	ILE	89	25.552	1.786	47.636	1.00	32.98	B
ATOM	570	O	ILE	89	24.485	2.243	48.016	1.00	33.67	B
ATOM	571	N	LEU	90	26.258	2.341	46.662	1.00	32.32	B
ATOM	572	CA	LEU	90	25.782	3.540	45.996	1.00	32.57	B
ATOM	573	CB	LEU	90	26.866	4.097	45.074	1.00	30.54	B
ATOM	574	CG	LEU	90	26.431	5.292	44.229	1.00	29.69	B
ATOM	575	CD1	LEU	90	26.018	6.448	45.122	1.00	28.62	B

ATOM	576	CD2	LEU	90	27.564	5.695	43.319	1.00	31.53	B
ATOM	577	C	LEU	90	24.504	3.272	45.202	1.00	32.92	B
ATOM	578	O	LEU	90	23.567	4.074	45.240	1.00	32.45	B
ATOM	579	N	ASP	91	24.466	2.147	44.491	1.00	33.45	B
ATOM	580	CA	ASP	91	23.292	1.785	43.699	1.00	34.72	B
ATOM	581	CB	ASP	91	23.520	0.470	42.940	1.00	35.65	B
ATOM	582	CG	ASP	91	24.593	0.582	41.863	1.00	39.61	B
ATOM	583	OD1	ASP	91	24.686	1.648	41.214	1.00	40.33	B
ATOM	584	OD2	ASP	91	25.335	-0.409	41.661	1.00	41.38	B
ATOM	585	C	ASP	91	22.068	1.633	44.597	1.00	33.10	B
ATOM	586	O	ASP	91	20.954	1.885	44.174	1.00	33.56	B
ATOM	587	N	GLU	92	22.290	1.221	45.839	1.00	32.56	B
ATOM	588	CA	GLU	92	21.196	1.044	46.783	1.00	34.16	B
ATOM	589	CB	GLU	92	21.657	0.171	47.954	1.00	37.44	B
ATOM	590	CG	GLU	92	20.545	-0.258	48.890	1.00	42.74	B
ATOM	591	CD	GLU	92	20.880	-1.536	49.648	1.00	46.50	B
ATOM	592	OE1	GLU	92	20.053	-1.956	50.490	1.00	47.07	B
ATOM	593	OE2	GLU	92	21.962	-2.120	49.396	1.00	46.74	B
ATOM	594	C	GLU	92	20.709	2.409	47.280	1.00	32.53	B
ATOM	595	O	GLU	92	19.518	2.608	47.519	1.00	30.70	B
ATOM	596	N	VAL	93	21.641	3.348	47.422	1.00	31.20	B
ATOM	597	CA	VAL	93	21.303	4.699	47.854	1.00	31.28	B
ATOM	598	CB	VAL	93	22.580	5.569	48.076	1.00	31.49	B
ATOM	599	CG1	VAL	93	22.194	7.010	48.365	1.00	27.40	B
ATOM	600	CG2	VAL	93	23.398	5.004	49.233	1.00	33.28	B
ATOM	601	C	VAL	93	20.452	5.322	46.750	1.00	29.79	B
ATOM	602	O	VAL	93	19.416	5.913	47.013	1.00	28.28	B
ATOM	603	N	ILE	94	20.899	5.163	45.510	1.00	27.82	B
ATOM	604	CA	ILE	94	20.166	5.703	44.378	1.00	30.44	B
ATOM	605	CB	ILE	94	20.915	5.429	43.051	1.00	28.59	B
ATOM	606	CG2	ILE	94	20.035	5.787	41.853	1.00	26.78	B
ATOM	607	CG1	ILE	94	22.216	6.240	43.037	1.00	27.01	B
ATOM	608	CD1	ILE	94	23.087	5.978	41.846	1.00	26.60	B
ATOM	609	C	ILE	94	18.749	5.131	44.306	1.00	32.32	B
ATOM	610	O	ILE	94	17.872	5.738	43.714	1.00	32.23	B
ATOM	611	N	MET	95	18.531	3.968	44.920	1.00	34.51	B
ATOM	612	CA	MET	95	17.201	3.360	44.923	1.00	36.17	B
ATOM	613	CB	MET	95	17.282	1.850	45.149	1.00	38.61	B
ATOM	614	CG	MET	95	17.372	1.017	43.881	1.00	40.44	B
ATOM	615	SD	MET	95	17.488	-0.772	44.242	1.00	46.46	B
ATOM	616	CE	MET	95	19.102	-1.171	43.546	1.00	44.51	B
ATOM	617	C	MET	95	16.315	3.979	45.996	1.00	36.50	B
ATOM	618	O	MET	95	15.113	3.732	46.030	1.00	37.42	B
ATOM	619	N	GLY	96	16.914	4.775	46.879	1.00	36.28	B
ATOM	620	CA	GLY	96	16.145	5.414	47.932	1.00	35.74	B
ATOM	621	C	GLY	96	16.366	4.830	49.314	1.00	36.78	B
ATOM	622	O	GLY	96	15.538	5.026	50.210	1.00	37.90	B
ATOM	623	N	TYR	97	17.479	4.118	49.487	1.00	36.85	B
ATOM	624	CA	TYR	97	17.835	3.496	50.763	1.00	37.58	B
ATOM	625	CB	TYR	97	18.381	2.081	50.525	1.00	40.65	B
ATOM	626	CG	TYR	97	17.341	1.025	50.217	1.00	45.13	B
ATOM	627	CD1	TYR	97	16.518	0.518	51.220	1.00	46.62	B
ATOM	628	CE1	TYR	97	15.558	-0.454	50.944	1.00	49.26	B
ATOM	629	CD2	TYR	97	17.182	0.533	48.921	1.00	46.06	B
ATOM	630	CE2	TYR	97	16.228	-0.436	48.630	1.00	49.09	B
ATOM	631	CZ	TYR	97	15.417	-0.928	49.646	1.00	50.42	B
ATOM	632	OH	TYR	97	14.465	-1.888	49.358	1.00	52.50	B
ATOM	633	C	TYR	97	18.889	4.304	51.526	1.00	35.44	B
ATOM	634	O	TYR	97	19.789	4.876	50.926	1.00	37.02	B
ATOM	635	N	ASN	98	18.776	4.349	52.849	1.00	31.97	B
ATOM	636	CA	ASN	98	19.759	5.059	53.662	1.00	30.42	B
ATOM	637	CB	ASN	98	19.169	5.460	55.025	1.00	30.64	B
ATOM	638	CG	ASN	98	18.239	6.663	54.945	1.00	28.74	B
ATOM	639	OD1	ASN	98	18.255	7.413	53.981	1.00	29.47	B
ATOM	640	ND2	ASN	98	17.436	6.855	55.984	1.00	27.34	B
ATOM	641	C	ASN	98	20.942	4.124	53.897	1.00	29.81	B
ATOM	642	O	ASN	98	20.762	3.006	54.324	1.00	29.82	B
ATOM	643	N	CYS	99	22.152	4.590	53.615	1.00	28.53	B
ATOM	644	CA	CYS	99	23.339	3.767	53.816	1.00	26.90	B
ATOM	645	CB	CYS	99	23.974	3.384	52.477	1.00	28.87	B
ATOM	646	SG	CYS	99	22.946	2.349	51.428	1.00	34.21	B
ATOM	647	C	CYS	99	24.382	4.465	54.677	1.00	25.00	B
ATOM	648	O	CYS	99	24.380	5.670	54.830	1.00	25.25	B

ATOM	649	N	THR	100	25.285	3.671	55.232	1.00	23.32	B
ATOM	650	CA	THR	100	26.341	4.187	56.080	1.00	19.59	B
ATOM	651	CB	THR	100	25.876	4.258	57.544	1.00	17.10	B
ATOM	652	OG1	THR	100	24.789	5.179	57.657	1.00	16.21	B
ATOM	653	CG2	THR	100	27.005	4.696	58.456	1.00	15.27	B
ATOM	654	C	THR	100	27.552	3.266	55.982	1.00	21.18	B
ATOM	655	O	THR	100	27.417	2.039	56.005	1.00	22.70	B
ATOM	656	N	ILE	101	28.732	3.858	55.849	1.00	18.53	B
ATOM	657	CA	ILE	101	29.967	3.097	55.782	1.00	17.55	B
ATOM	658	CB	ILE	101	30.650	3.212	54.420	1.00	16.14	B
ATOM	659	CG2	ILE	101	31.939	2.414	54.423	1.00	16.50	B
ATOM	660	CG1	ILE	101	29.730	2.690	53.318	1.00	14.57	B
ATOM	661	CD1	ILE	101	30.186	3.077	51.930	1.00	14.45	B
ATOM	662	C	ILE	101	30.913	3.654	56.834	1.00	19.99	B
ATOM	663	O	ILE	101	31.296	4.822	56.786	1.00	20.78	B
ATOM	664	N	PHE	102	31.273	2.808	57.793	1.00	19.14	B
ATOM	665	CA	PHE	102	32.176	3.179	58.876	1.00	17.58	B
ATOM	666	CB	PHE	102	31.835	2.373	60.123	1.00	17.67	B
ATOM	667	CG	PHE	102	30.618	2.842	60.847	1.00	17.05	B
ATOM	668	CD1	PHE	102	30.714	3.855	61.790	1.00	16.04	B
ATOM	669	CD2	PHE	102	29.386	2.239	60.624	1.00	16.40	B
ATOM	670	CE1	PHE	102	29.603	4.265	62.508	1.00	16.56	B
ATOM	671	CE2	PHE	102	28.268	2.643	61.337	1.00	18.62	B
ATOM	672	CZ	PHE	102	28.377	3.658	62.283	1.00	16.81	B
ATOM	673	C	PHE	102	33.625	2.891	58.515	1.00	16.69	B
ATOM	674	O	PHE	102	33.910	2.289	57.516	1.00	18.17	B
ATOM	675	N	ALA	103	34.535	3.338	59.366	1.00	17.68	B
ATOM	676	CA	ALA	103	35.961	3.089	59.187	1.00	17.02	B
ATOM	677	CB	ALA	103	36.620	4.229	58.451	1.00	16.82	B
ATOM	678	C	ALA	103	36.471	2.991	60.617	1.00	17.64	B
ATOM	679	O	ALA	103	36.482	3.963	61.339	1.00	18.79	B
ATOM	680	N	TYR	104	36.866	1.786	61.012	1.00	18.22	B
ATOM	681	CA	TYR	104	37.340	1.540	62.368	1.00	16.40	B
ATOM	682	CB	TYR	104	36.436	0.496	63.034	1.00	15.83	B
ATOM	683	CG	TYR	104	36.706	0.291	64.508	1.00	12.67	B
ATOM	684	CD1	TYR	104	37.771	-0.501	64.941	1.00	10.95	B
ATOM	685	CE1	TYR	104	38.046	-0.659	66.301	1.00	11.52	B
ATOM	686	CD2	TYR	104	35.919	0.920	65.469	1.00	10.91	B
ATOM	687	CE2	TYR	104	36.187	0.768	66.832	1.00	12.42	B
ATOM	688	CZ	TYR	104	37.253	-0.023	67.239	1.00	10.32	B
ATOM	689	OH	TYR	104	37.526	-0.180	68.574	1.00	11.99	B
ATOM	690	C	TYR	104	38.778	1.061	62.380	1.00	15.64	B
ATOM	691	O	TYR	104	39.203	0.348	61.497	1.00	17.51	B
ATOM	692	N	GLY	105	39.524	1.456	63.397	1.00	15.78	B
ATOM	693	CA	GLY	105	40.904	1.047	63.475	1.00	16.05	B
ATOM	694	C	GLY	105	41.748	2.044	64.226	1.00	16.81	B
ATOM	695	O	GLY	105	41.318	3.151	64.526	1.00	19.22	B
ATOM	696	N	GLN	106	42.963	1.616	64.531	1.00	18.16	B
ATOM	697	CA	GLN	106	43.940	2.408	65.244	1.00	18.74	B
ATOM	698	CB	GLN	106	45.122	1.519	65.652	1.00	19.69	B
ATOM	699	CG	GLN	106	46.278	2.251	66.305	1.00	23.87	B
ATOM	700	CD	GLN	106	47.527	1.411	66.407	1.00	24.14	B
ATOM	701	OE1	GLN	106	47.865	0.669	65.490	1.00	27.37	B
ATOM	702	NE2	GLN	106	48.225	1.528	67.525	1.00	25.29	B
ATOM	703	C	GLN	106	44.440	3.552	64.363	1.00	20.10	B
ATOM	704	O	GLN	106	44.438	3.451	63.134	1.00	19.09	B
ATOM	705	N	THR	107	44.864	4.639	65.004	1.00	19.11	B
ATOM	706	CA	THR	107	45.385	5.792	64.291	1.00	18.65	B
ATOM	707	CB	THR	107	45.849	6.914	65.270	1.00	20.97	B
ATOM	708	OG1	THR	107	44.730	7.405	66.017	1.00	19.66	B
ATOM	709	CG2	THR	107	46.476	8.064	64.497	1.00	15.96	B
ATOM	710	C	THR	107	46.588	5.391	63.439	1.00	17.71	B
ATOM	711	O	THR	107	47.518	4.747	63.921	1.00	16.56	B
ATOM	712	N	GLY	108	46.554	5.786	62.171	1.00	17.28	B
ATOM	713	CA	GLY	108	47.642	5.483	61.267	1.00	15.71	B
ATOM	714	C	GLY	108	47.499	4.181	60.505	1.00	17.55	B
ATOM	715	O	GLY	108	48.489	3.682	59.938	1.00	17.87	B
ATOM	716	N	THR	109	46.288	3.626	60.478	1.00	15.83	B
ATOM	717	CA	THR	109	46.064	2.374	59.765	1.00	14.74	B
ATOM	718	CB	THR	109	45.276	1.352	60.632	1.00	13.57	B
ATOM	719	OG1	THR	109	43.978	1.866	60.943	1.00	13.63	B
ATOM	720	CG2	THR	109	46.035	1.064	61.934	1.00	12.00	B
ATOM	721	C	THR	109	45.350	2.573	58.435	1.00	15.88	B

ATOM	722	O	THR	109	45.132	1.602	57.708	1.00	14.55	B	
ATOM	723	N	GLY	110	44.977	3.819	58.124	1.00	13.70	B	
ATOM	724	CA	GLY	110	44.321	4.073	56.849	1.00	10.56	B	
ATOM	725	C	GLY	110	42.846	4.433	56.833	1.00	10.76	B	
ATOM	726	O	GLY	110	42.201	4.298	55.792	1.00	9.95	B	
ATOM	727	N	LYS	111	42.302	4.885	57.959	1.00	8.99	B	
ATOM	728	CA	LYS	111	40.889	5.267	58.022	1.00	11.48	B	
ATOM	729	CB	LYS	111	40.497	5.693	59.449	1.00	12.59	B	
ATOM	730	CG	LYS	111	40.315	4.531	60.426	1.00	15.28	B	
ATOM	731	CD	LYS	111	39.651	4.955	61.738	1.00	12.73	B	
ATOM	732	CE	LYS	111	40.439	6.034	62.455	1.00	11.56	B	
ATOM	733	NZ	LYS	111	41.905	5.766	62.396	1.00	10.51	B	
ATOM	734	C	LYS	111	40.575	6.408	57.062	1.00	13.97	B	
ATOM	735	O	LYS	111	39.683	6.302	56.206	1.00	15.37	B	
ATOM	736	N	THR	112	41.321	7.498	57.198	1.00	13.82	B	
ATOM	737	CA	THR	112	41.120	8.663	56.353	1.00	12.58	B	
ATOM	738	CB	THR	112	41.895	9.871	56.926	1.00	12.79	B	
ATOM	739	OG1	THR	112	41.408	10.160	58.245	1.00	9.63	B	
ATOM	740	CG2	THR	112	41.723	11.103	56.037	1.00	10.46	B	
ATOM	741	C	THR	112	41.535	8.396	54.905	1.00	14.40	B	
ATOM	742	O	THR	112	40.886	8.846	53.978	1.00	15.19	B	
ATOM	743	N	PHE	113	42.618	7.651	54.723	1.00	15.74	B	
ATOM	744	CA	PHE	113	43.095	7.326	53.384	1.00	17.09	B	
ATOM	745	CB	PHE	113	44.316	6.408	53.463	1.00	17.69	B	
ATOM	746	CG	PHE	113	44.867	6.030	52.123	1.00	20.87	B	
ATOM	747	CD1	PHE	113	45.783	6.849	51.475	1.00	22.41	B	
ATOM	748	CD2	PHE	113	44.445	4.871	51.490	1.00	22.63	B	
ATOM	749	CE1	PHE	113	46.271	6.517	50.218	1.00	22.81	B	
ATOM	750	CE2	PHE	113	44.924	4.529	50.228	1.00	23.87	B	
ATOM	751	CZ	PHE	113	45.840	5.354	49.590	1.00	25.27	B	
ATOM	752	C	PHE	113	42.000	6.626	52.580	1.00	18.62	B	
ATOM	753	O	PHE	113	41.817	6.888	51.389	1.00	17.60	B	
ATOM	754	N	THR	114	41.291	5.719	53.247	1.00	19.63	B	
ATOM	755	CA	THR	114	40.212	4.945	52.646	1.00	18.57	B	
ATOM	756	CB	THR	114	39.816	3.760	53.582	1.00	20.30	B	
ATOM	757	OG1	THR	114	40.970	2.947	53.828	1.00	18.79	B	
ATOM	758	CG2	THR	114	38.700	2.910	52.972	1.00	12.74	B	
ATOM	759	C	THR	114	38.991	5.825	52.410	1.00	19.70	B	
ATOM	760	O	THR	114	38.497	5.932	51.297	1.00	22.13	B	
ATOM	761	N	MET	115	38.518	6.473	53.465	1.00	19.43	B	
ATOM	762	CA	MET	115	37.345	7.318	53.347	1.00	20.55	B	
ATOM	763	CB	MET	115	36.877	7.771	54.730	1.00	21.97	B	
ATOM	764	CG	MET	115	36.471	6.620	55.644	1.00	27.07	B	
ATOM	765	SD	MET	115	35.328	5.432	54.848	1.00	29.66	B	
ATOM	766	CE	MET	115	33.753	6.265	55.089	1.00	27.98	B	
ATOM	767	C	MET	115	37.532	8.528	52.454	1.00	21.26	B	
ATOM	768	O	MET	115	36.639	8.866	51.674	1.00	23.74	B	
ATOM	769	N	GLU	116	38.687	9.179	52.549	1.00	20.10	B	
ATOM	770	CA	GLU	116	38.937	10.377	51.749	1.00	20.30	B	
ATOM	771	CB	GLU	116	39.323	11.541	52.659	1.00	19.03	B	
ATOM	772	CG	GLU	116	38.309	11.824	53.741	1.00	17.09	B	
ATOM	773	CD	GLU	116	38.746	12.922	54.687	1.00	18.90	B	
ATOM	774	OE1	GLU	116	39.886	13.421	54.550	1.00	21.39	B	
ATOM	775	OE2	GLU	116	37.951	13.280	55.579	1.00	17.52	B	
ATOM	776	C	GLU	116	40.010	10.194	50.694	1.00	20.60	B	
ATOM	777	O	GLU	116	39.804	10.494	49.527	1.00	19.26	B	
ATOM	778	N	GLY	117	41.166	9.708	51.116	1.00	22.39	B	
ATOM	779	CA	GLY	117	42.249	9.508	50.176	1.00	24.67	B	
ATOM	780	C	GLY	117	43.194	10.689	50.144	1.00	25.76	B	
ATOM	781	O	GLY	117	43.056	11.630	50.918	1.00	24.17	B	
ATOM	782	N	GLU	118	44.162	10.635	49.237	1.00	27.49	B	
ATOM	783	CA	GLU	118	45.133	11.710	49.128	1.00	28.73	B	
ATOM	784	CB	GLU	118	46.465	11.273	49.740	1.00	30.64	B	
ATOM	785	CG	GLU	118	46.311	10.255	50.853	1.00	35.23	B	
ATOM	786	CD	GLU	118	47.579	10.060	51.657	1.00	37.43	B	
ATOM	787	OE1	GLU	118	48.671	9.993	51.049	1.00	35.58	B	
ATOM	788	OE2	GLU	118	47.476	9.958	52.900	1.00	40.04	B	
ATOM	789	C	GLU	118	45.338	12.082	47.671	1.00	27.97	B	
ATOM	790	O	GLU	118	44.692	11.542	46.779	1.00	29.50	B	
ATOM	791	N	ARG	119	46.244	13.017	47.436	1.00	25.87	B	
ATOM	792	CA	ARG	119	46.532	13.439	46.085	1.00	25.52	B	
ATOM	793	CB	ARG	119	46.613	14.968	46.006	1.00	24.48	B	
ATOM	794	CG	ARG	119	45.323	15.708	46.358	1.00	23.62	B	

ATOM	795	CD	ARG	119	44.190	15.361	45.387	1.00	22.16	B
ATOM	796	NE	ARG	119	44.654	15.191	44.011	1.00	20.25	B
ATOM	797	CZ	ARG	119	44.382	16.018	43.005	1.00	19.31	B
ATOM	798	NH1	ARG	119	43.642	17.102	43.203	1.00	19.24	B
ATOM	799	NH2	ARG	119	44.842	15.744	41.791	1.00	17.50	B
ATOM	800	C	ARG	119	47.857	12.836	45.654	1.00	26.80	B
ATOM	801	O	ARG	119	48.779	12.711	46.457	1.00	25.89	B
ATOM	802	N	SER	120	47.942	12.440	44.390	1.00	25.98	B
ATOM	803	CA	SER	120	49.189	11.893	43.880	1.00	28.78	B
ATOM	804	CB	SER	120	49.015	11.326	42.472	1.00	29.79	B
ATOM	805	OG	SER	120	48.428	10.038	42.508	1.00	33.26	B
ATOM	806	C	SER	120	50.130	13.077	43.834	1.00	27.18	B
ATOM	807	O	SER	120	49.779	14.121	43.326	1.00	27.97	B
ATOM	808	N	PRO	121	51.348	12.913	44.357	1.00	27.06	B
ATOM	809	CD	PRO	121	51.902	11.662	44.900	1.00	26.17	B
ATOM	810	CA	PRO	121	52.350	13.987	44.381	1.00	27.66	B
ATOM	811	CB	PRO	121	53.528	13.342	45.117	1.00	27.55	B
ATOM	812	CG	PRO	121	53.386	11.899	44.779	1.00	28.94	B
ATOM	813	C	PRO	121	52.760	14.591	43.031	1.00	27.47	B
ATOM	814	O	PRO	121	52.773	13.914	42.009	1.00	27.14	B
ATOM	815	N	ASN	122	53.072	15.885	43.050	1.00	27.34	B
ATOM	816	CA	ASN	122	53.517	16.615	41.865	1.00	28.41	B
ATOM	817	CB	ASN	122	54.690	15.875	41.217	1.00	29.21	B
ATOM	818	CG	ASN	122	55.857	16.789	40.906	1.00	29.30	B
ATOM	819	OD1	ASN	122	56.355	17.491	41.777	1.00	30.37	B
ATOM	820	ND2	ASN	122	56.305	16.774	39.656	1.00	30.61	B
ATOM	821	C	ASN	122	52.434	16.859	40.817	1.00	28.67	B
ATOM	822	O	ASN	122	52.725	16.940	39.627	1.00	25.87	B
ATOM	823	N	GLU	123	51.191	16.985	41.265	1.00	30.12	B
ATOM	824	CA	GLU	123	50.070	17.240	40.356	1.00	33.32	B
ATOM	825	CB	GLU	123	50.105	18.699	39.870	1.00	33.54	B
ATOM	826	CG	GLU	123	50.037	19.748	40.968	1.00	33.76	B
ATOM	827	CD	GLU	123	49.872	21.158	40.420	1.00	34.11	B
ATOM	828	OE1	GLU	123	50.763	21.623	39.678	1.00	32.71	B
ATOM	829	OE2	GLU	123	48.848	21.804	40.734	1.00	33.32	B
ATOM	830	C	GLU	123	50.061	16.307	39.137	1.00	34.30	B
ATOM	831	O	GLU	123	49.856	16.743	38.013	1.00	32.10	B
ATOM	832	N	GLU	124	50.283	15.020	39.373	1.00	36.35	B
ATOM	833	CA	GLU	124	50.303	14.046	38.292	1.00	36.52	B
ATOM	834	CB	GLU	124	50.709	12.678	38.846	1.00	40.35	B
ATOM	835	CG	GLU	124	51.279	11.711	37.815	1.00	45.05	B
ATOM	836	CD	GLU	124	52.026	10.550	38.458	1.00	47.77	B
ATOM	837	OE1	GLU	124	51.966	10.427	39.705	1.00	47.83	B
ATOM	838	OE2	GLU	124	52.671	9.769	37.720	1.00	48.04	B
ATOM	839	C	GLU	124	48.942	13.964	37.590	1.00	36.15	B
ATOM	840	O	GLU	124	48.876	13.987	36.363	1.00	34.16	B
ATOM	841	N	TYR	125	47.859	13.886	38.361	1.00	35.31	B
ATOM	842	CA	TYR	125	46.524	13.803	37.770	1.00	36.12	B
ATOM	843	CB	TYR	125	45.863	12.440	38.054	1.00	38.61	B
ATOM	844	CG	TYR	125	46.757	11.216	37.992	1.00	39.31	B
ATOM	845	CD1	TYR	125	47.657	10.933	39.019	1.00	39.77	B
ATOM	846	CE1	TYR	125	48.454	9.784	38.987	1.00	40.96	B
ATOM	847	CD2	TYR	125	46.675	10.321	36.922	1.00	39.64	B
ATOM	848	CE2	TYR	125	47.468	9.169	36.879	1.00	40.42	B
ATOM	849	CZ	TYR	125	48.355	8.908	37.916	1.00	41.60	B
ATOM	850	OH	TYR	125	49.141	7.776	37.882	1.00	43.64	B
ATOM	851	C	TYR	125	45.590	14.873	38.332	1.00	35.75	B
ATOM	852	O	TYR	125	45.925	15.577	39.273	1.00	36.04	B
ATOM	853	N	THR	126	44.409	14.976	37.729	1.00	35.01	B
ATOM	854	CA	THR	126	43.385	15.901	38.189	1.00	34.12	B
ATOM	855	CB	THR	126	42.393	16.275	37.064	1.00	34.09	B
ATOM	856	OG1	THR	126	41.885	15.080	36.458	1.00	36.33	B
ATOM	857	CG2	THR	126	43.075	17.134	36.005	1.00	30.16	B
ATOM	858	C	THR	126	42.645	15.117	39.271	1.00	34.15	B
ATOM	859	O	THR	126	42.555	13.896	39.197	1.00	35.30	B
ATOM	860	N	TRP	127	42.111	15.807	40.270	1.00	33.25	B
ATOM	861	CA	TRP	127	41.422	15.133	41.363	1.00	31.64	B
ATOM	862	CB	TRP	127	40.596	16.135	42.182	1.00	28.58	B
ATOM	863	CG	TRP	127	39.362	16.610	41.489	1.00	25.55	B
ATOM	864	CD2	TRP	127	38.066	16.008	41.551	1.00	23.28	B
ATOM	865	CE2	TRP	127	37.218	16.754	40.699	1.00	23.64	B
ATOM	866	CE3	TRP	127	37.537	14.907	42.244	1.00	23.43	B
ATOM	867	CD1	TRP	127	39.255	17.667	40.631	1.00	23.80	B

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ATOM    868  NE1 TRP   127      37.969  17.761  40.150  1.00 24.71      B
ATOM    869  CZ2 TRP   127      35.867  16.433  40.518  1.00 24.05      B
ATOM    870  CZ3 TRP   127      36.192  14.585  42.065  1.00 24.74      B
ATOM    871  CH2 TRP   127      35.372  15.351  41.207  1.00 26.04      B
ATOM    872  C   TRP   127      40.522  13.968  40.931  1.00 31.94      B
ATOM    873  O   TRP   127      40.510  12.927  41.579  1.00 32.64      B
ATOM    874  N   GLU   128      39.781  14.131  39.838  1.00 32.66      B
ATOM    875  CA  GLU   128      38.869  13.078  39.394  1.00 33.32      B
ATOM    876  CB  GLU   128      37.785  13.669  38.502  1.00 34.68      B
ATOM    877  CG  GLU   128      38.287  14.201  37.178  1.00 39.01      B
ATOM    878  CD  GLU   128      37.206  14.964  36.442  1.00 42.74      B
ATOM    879  OE1 GLU   128      36.895  16.100  36.867  1.00 44.33      B
ATOM    880  OE2 GLU   128      36.654  14.422  35.458  1.00 43.63      B
ATOM    881  C   GLU   128      39.512  11.879  38.700  1.00 32.67      B
ATOM    882  O   GLU   128      38.825  10.930  38.348  1.00 31.45      B
ATOM    883  N   GLU   129      40.825  11.926  38.500  1.00 32.62      B
ATOM    884  CA  GLU   129      41.532  10.815  37.871  1.00 33.28      B
ATOM    885  CB  GLU   129      42.192  11.246  36.561  1.00 35.75      B
ATOM    886  CG  GLU   129      41.218  11.496  35.420  1.00 39.64      B
ATOM    887  CD  GLU   129      41.922  11.680  34.082  1.00 42.49      B
ATOM    888  OE1 GLU   129      41.266  12.139  33.119  1.00 43.56      B
ATOM    889  OE2 GLU   129      43.129  11.367  33.996  1.00 45.44      B
ATOM    890  C   GLU   129      42.602  10.280  38.808  1.00 33.23      B
ATOM    891  O   GLU   129      43.242   9.297  38.511  1.00 33.33      B
ATOM    892  N   ASP   130      42.776  10.934  39.951  1.00 32.98      B
ATOM    893  CA  ASP   130      43.789  10.516  40.912  1.00 32.86      B
ATOM    894  CB  ASP   130      43.884  11.544  42.045  1.00 34.15      B
ATOM    895  CG  ASP   130      45.247  11.564  42.699  1.00 35.32      B
ATOM    896  OD1 ASP   130      45.765  10.477  43.030  1.00 36.91      B
ATOM    897  OD2 ASP   130      45.801  12.665  42.882  1.00 36.83      B
ATOM    898  C   ASP   130      43.468   9.129  41.485  1.00 33.07      B
ATOM    899  O   ASP   130      42.429   8.928  42.114  1.00 32.52      B
ATOM    900  N   PRO   131      44.367   8.152  41.268  1.00 32.43      B
ATOM    901  CD  PRO   131      45.638   8.278  40.533  1.00 32.63      B
ATOM    902  CA  PRO   131      44.186   6.782  41.757  1.00 30.77      B
ATOM    903  CB  PRO   131      45.339   6.029  41.102  1.00 31.15      B
ATOM    904  CG  PRO   131      46.399   7.073  41.005  1.00 31.37      B
ATOM    905  C   PRO   131      44.192   6.673  43.283  1.00 30.54      B
ATOM    906  O   PRO   131      43.717   5.688  43.845  1.00 31.07      B
ATOM    907  N   LEU   132      44.721   7.691  43.953  1.00 28.68      B
ATOM    908  CA  LEU   132      44.750   7.684  45.407  1.00 26.49      B
ATOM    909  CB  LEU   132      45.965   8.461  45.918  1.00 24.68      B
ATOM    910  CG  LEU   132      47.355   7.961  45.497  1.00 25.57      B
ATOM    911  CD1 LEU   132      48.414   8.782  46.221  1.00 24.29      B
ATOM    912  CD2 LEU   132      47.526   6.481  45.843  1.00 26.94      B
ATOM    913  C   LEU   132      43.455   8.248  46.008  1.00 26.30      B
ATOM    914  O   LEU   132      43.294   8.285  47.228  1.00 26.84      B
ATOM    915  N   ALA   133      42.532   8.672  45.145  1.00 24.55      B
ATOM    916  CA  ALA   133      41.243   9.217  45.572  1.00 25.15      B
ATOM    917  CB  ALA   133      40.393   9.562  44.352  1.00 24.26      B
ATOM    918  C   ALA   133      40.502   8.215  46.453  1.00 25.64      B
ATOM    919  O   ALA   133      40.528   7.034  46.201  1.00 27.86      B
ATOM    920  N   GLY   134      39.831   8.706  47.485  1.00 26.27      B
ATOM    921  CA  GLY   134      39.107   7.822  48.379  1.00 24.63      B
ATOM    922  C   GLY   134      37.633   7.705  48.038  1.00 24.63      B
ATOM    923  O   GLY   134      37.176   8.224  47.013  1.00 23.91      B
ATOM    924  N   ILE   135      36.887   7.030  48.910  1.00 22.69      B
ATOM    925  CA  ILE   135      35.457   6.816  48.704  1.00 21.86      B
ATOM    926  CB  ILE   135      34.839   6.028  49.898  1.00 21.68      B
ATOM    927  CG2 ILE   135      33.315   5.945  49.745  1.00 20.01      B
ATOM    928  CG1 ILE   135      35.464   4.628  49.971  1.00 20.31      B
ATOM    929  CD1 ILE   135      35.183   3.865  51.246  1.00 16.89      B
ATOM    930  C   ILE   135      34.652   8.103  48.481  1.00 20.87      B
ATOM    931  O   ILE   135      33.956   8.228  47.495  1.00 19.45      B
ATOM    932  N   ILE   136      34.762   9.053  49.405  1.00 20.74      B
ATOM    933  CA  ILE   136      34.018  10.309  49.297  1.00 19.78      B
ATOM    934  CB  ILE   136      34.420  11.273  50.436  1.00 19.46      B
ATOM    935  CG2 ILE   136      33.654  12.581  50.302  1.00 23.46      B
ATOM    936  CG1 ILE   136      34.128  10.616  51.792  1.00 19.18      B
ATOM    937  CD1 ILE   136      34.597  11.398  53.011  1.00 20.13      B
ATOM    938  C   ILE   136      34.146  11.016  47.929  1.00 19.32      B
ATOM    939  O   ILE   136      33.149  11.258  47.255  1.00 18.78      B
ATOM    940  N   PRO   137      35.377  11.340  47.499  1.00 18.18      B
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ATOM	941	CD	PRO	137	36.695	11.158	48.127	1.00	15.47	B
ATOM	942	CA	PRO	137	35.501	12.008	46.198	1.00	17.79	B
ATOM	943	CB	PRO	137	36.995	12.321	46.105	1.00	15.58	B
ATOM	944	CG	PRO	137	37.618	11.255	46.946	1.00	16.71	B
ATOM	945	C	PRO	137	35.010	11.135	45.040	1.00	20.22	B
ATOM	946	O	PRO	137	34.434	11.625	44.080	1.00	21.41	B
ATOM	947	N	ARG	138	35.234	9.829	45.135	1.00	22.72	B
ATOM	948	CA	ARG	138	34.789	8.927	44.075	1.00	22.41	B
ATOM	949	CB	ARG	138	35.378	7.534	44.270	1.00	21.69	B
ATOM	950	CG	ARG	138	36.860	7.433	43.951	1.00	20.35	B
ATOM	951	CD	ARG	138	37.395	6.072	44.347	1.00	17.89	B
ATOM	952	NE	ARG	138	38.847	6.020	44.275	1.00	17.83	B
ATOM	953	CZ	ARG	138	39.529	5.905	43.142	1.00	18.07	B
ATOM	954	NH1	ARG	138	38.886	5.818	41.987	1.00	19.38	B
ATOM	955	NH2	ARG	138	40.854	5.906	43.156	1.00	18.54	B
ATOM	956	C	ARG	138	33.263	8.829	44.007	1.00	22.14	B
ATOM	957	O	ARG	138	32.689	8.890	42.942	1.00	23.68	B
ATOM	958	N	THR	139	32.615	8.678	45.154	1.00	22.12	B
ATOM	959	CA	THR	139	31.161	8.566	45.203	1.00	25.57	B
ATOM	960	CB	THR	139	30.675	8.360	46.662	1.00	25.67	B
ATOM	961	OG1	THR	139	31.355	7.236	47.234	1.00	27.07	B
ATOM	962	CG2	THR	139	29.174	8.100	46.700	1.00	27.35	B
ATOM	963	C	THR	139	30.463	9.797	44.614	1.00	26.55	B
ATOM	964	O	THR	139	29.544	9.675	43.809	1.00	26.69	B
ATOM	965	N	LEU	140	30.910	10.982	45.017	1.00	27.11	B
ATOM	966	CA	LEU	140	30.314	12.213	44.523	1.00	26.17	B
ATOM	967	CB	LEU	140	30.949	13.424	45.209	1.00	26.20	B
ATOM	968	CG	LEU	140	30.599	13.605	46.690	1.00	26.65	B
ATOM	969	CD1	LEU	140	31.435	14.723	47.280	1.00	25.28	B
ATOM	970	CD2	LEU	140	29.114	13.896	46.849	1.00	24.93	B
ATOM	971	C	LEU	140	30.473	12.320	43.018	1.00	25.73	B
ATOM	972	O	LEU	140	29.556	12.725	42.333	1.00	25.93	B
ATOM	973	N	HIS	141	31.641	11.941	42.514	1.00	25.67	B
ATOM	974	CA	HIS	141	31.907	12.001	41.081	1.00	26.55	B
ATOM	975	CB	HIS	141	33.394	11.743	40.813	1.00	25.96	B
ATOM	976	CG	HIS	141	33.770	11.804	39.364	1.00	26.57	B
ATOM	977	CD2	HIS	141	33.823	10.841	38.415	1.00	28.59	B
ATOM	978	ND1	HIS	141	34.138	12.974	38.739	1.00	29.67	B
ATOM	979	CE1	HIS	141	34.405	12.731	37.467	1.00	29.67	B
ATOM	980	NE2	HIS	141	34.221	11.443	37.245	1.00	28.28	B
ATOM	981	C	HIS	141	31.072	10.973	40.322	1.00	26.86	B
ATOM	982	O	HIS	141	30.679	11.199	39.181	1.00	28.03	B
ATOM	983	N	GLN	142	30.802	9.844	40.965	1.00	24.80	B
ATOM	984	CA	GLN	142	30.045	8.780	40.326	1.00	25.14	B
ATOM	985	CB	GLN	142	30.353	7.436	40.994	1.00	27.48	B
ATOM	986	CG	GLN	142	31.680	6.834	40.563	1.00	30.52	B
ATOM	987	CD	GLN	142	31.684	6.417	39.102	1.00	34.29	B
ATOM	988	OE1	GLN	142	30.990	5.475	38.711	1.00	34.96	B
ATOM	989	NE2	GLN	142	32.468	7.116	38.287	1.00	35.49	B
ATOM	990	C	GLN	142	28.550	9.017	40.317	1.00	22.70	B
ATOM	991	O	GLN	142	27.856	8.528	39.440	1.00	21.46	B
ATOM	992	N	ILE	143	28.058	9.766	41.297	1.00	21.92	B
ATOM	993	CA	ILE	143	26.634	10.062	41.365	1.00	22.81	B
ATOM	994	CB	ILE	143	26.304	10.888	42.620	1.00	22.20	B
ATOM	995	CG2	ILE	143	24.880	11.423	42.533	1.00	22.62	B
ATOM	996	CG1	ILE	143	26.476	10.024	43.872	1.00	21.94	B
ATOM	997	CD1	ILE	143	26.390	10.793	45.177	1.00	20.22	B
ATOM	998	C	ILE	143	26.187	10.824	40.114	1.00	24.31	B
ATOM	999	O	ILE	143	25.156	10.525	39.544	1.00	24.61	B
ATOM	1000	N	PHE	144	26.987	11.803	39.693	1.00	26.83	B
ATOM	1001	CA	PHE	144	26.672	12.611	38.511	1.00	28.06	B
ATOM	1002	CB	PHE	144	27.580	13.857	38.439	1.00	26.87	B
ATOM	1003	CG	PHE	144	27.330	14.861	39.536	1.00	27.89	B
ATOM	1004	CD1	PHE	144	26.169	15.630	39.545	1.00	29.48	B
ATOM	1005	CD2	PHE	144	28.230	15.002	40.592	1.00	28.77	B
ATOM	1006	CE1	PHE	144	25.901	16.518	40.592	1.00	28.27	B
ATOM	1007	CE2	PHE	144	27.974	15.890	41.647	1.00	28.13	B
ATOM	1008	CZ	PHE	144	26.805	16.646	41.646	1.00	30.04	B
ATOM	1009	C	PHE	144	26.818	11.778	37.238	1.00	28.29	B
ATOM	1010	O	PHE	144	26.140	12.025	36.253	1.00	28.71	B
ATOM	1011	N	GLU	145	27.703	10.786	37.273	1.00	29.40	B
ATOM	1012	CA	GLU	145	27.915	9.909	36.122	1.00	31.01	B
ATOM	1013	CB	GLU	145	29.216	9.129	36.297	1.00	32.65	B

ATOM	1014	CG	GLU	145	30.467	9.938	36.056	1.00	38.99	B
ATOM	1015	CD	GLU	145	30.706	10.197	34.578	1.00	43.44	B
ATOM	1016	OE1	GLU	145	31.623	10.987	34.246	1.00	45.83	B
ATOM	1017	OE2	GLU	145	29.977	9.603	33.752	1.00	45.50	B
ATOM	1018	C	GLU	145	26.753	8.926	35.940	1.00	31.44	B
ATOM	1019	O	GLU	145	26.237	8.754	34.841	1.00	30.51	B
ATOM	1020	N	LYS	146	26.348	8.290	37.033	1.00	31.75	B
ATOM	1021	CA	LYS	146	25.269	7.310	37.012	1.00	33.61	B
ATOM	1022	CB	LYS	146	25.172	6.629	38.381	1.00	34.03	B
ATOM	1023	CG	LYS	146	26.350	5.717	38.695	1.00	38.09	B
ATOM	1024	CD	LYS	146	26.243	5.107	40.086	1.00	40.00	B
ATOM	1025	CE	LYS	146	27.228	3.958	40.263	1.00	43.91	B
ATOM	1026	NZ	LYS	146	26.919	2.818	39.352	1.00	43.76	B
ATOM	1027	C	LYS	146	23.908	7.882	36.624	1.00	33.97	B
ATOM	1028	O	LYS	146	23.171	7.276	35.840	1.00	33.52	B
ATOM	1029	N	LEU	147	23.577	9.046	37.176	1.00	33.52	B
ATOM	1030	CA	LEU	147	22.302	9.689	36.892	1.00	32.92	B
ATOM	1031	CB	LEU	147	21.746	10.320	38.175	1.00	31.38	B
ATOM	1032	CG	LEU	147	21.336	9.359	39.302	1.00	32.23	B
ATOM	1033	CD1	LEU	147	21.060	10.138	40.585	1.00	31.01	B
ATOM	1034	CD2	LEU	147	20.096	8.569	38.883	1.00	32.23	B
ATOM	1035	C	LEU	147	22.418	10.749	35.794	1.00	32.85	B
ATOM	1036	O	LEU	147	21.562	11.609	35.669	1.00	33.29	B
ATOM	1037	N	THR	148	23.475	10.666	34.992	1.00	33.48	B
ATOM	1038	CA	THR	148	23.701	11.636	33.921	1.00	35.96	B
ATOM	1039	CB	THR	148	24.900	11.236	33.036	1.00	36.22	B
ATOM	1040	OG1	THR	148	25.074	12.218	32.008	1.00	37.20	B
ATOM	1041	CG2	THR	148	24.664	9.871	32.381	1.00	38.66	B
ATOM	1042	C	THR	148	22.484	11.879	33.014	1.00	36.52	B
ATOM	1043	O	THR	148	22.123	13.021	32.772	1.00	35.06	B
ATOM	1044	N	ASP	149	21.868	10.806	32.514	1.00	35.79	B
ATOM	1045	CA	ASP	149	20.690	10.923	31.648	1.00	35.29	B
ATOM	1046	CB	ASP	149	21.101	11.265	30.206	1.00	36.06	B
ATOM	1047	CG	ASP	149	22.065	10.249	29.607	1.00	37.80	B
ATOM	1048	OD1	ASP	149	22.292	9.196	30.243	1.00	40.41	B
ATOM	1049	OD2	ASP	149	22.590	10.500	28.496	1.00	36.11	B
ATOM	1050	C	ASP	149	19.821	9.657	31.646	1.00	34.60	B
ATOM	1051	O	ASP	149	19.397	9.184	30.592	1.00	31.15	B
ATOM	1052	N	ASN	150	19.554	9.122	32.834	1.00	34.29	B
ATOM	1053	CA	ASN	150	18.732	7.923	32.948	1.00	35.52	B
ATOM	1054	CB	ASN	150	19.227	7.041	34.102	1.00	32.56	B
ATOM	1055	CG	ASN	150	19.031	7.690	35.452	1.00	32.34	B
ATOM	1056	OD1	ASN	150	19.134	8.903	35.579	1.00	29.46	B
ATOM	1057	ND2	ASN	150	18.760	6.877	36.475	1.00	31.14	B
ATOM	1058	C	ASN	150	17.265	8.292	33.154	1.00	36.96	B
ATOM	1059	O	ASN	150	16.436	7.431	33.447	1.00	37.74	B
ATOM	1060	N	GLY	151	16.953	9.578	32.996	1.00	37.37	B
ATOM	1061	CA	GLY	151	15.585	10.044	33.153	1.00	37.75	B
ATOM	1062	C	GLY	151	15.195	10.351	34.585	1.00	39.12	B
ATOM	1063	O	GLY	151	14.013	10.490	34.903	1.00	39.41	B
ATOM	1064	N	THR	152	16.190	10.455	35.455	1.00	40.74	B
ATOM	1065	CA	THR	152	15.950	10.748	36.860	1.00	42.40	B
ATOM	1066	CB	THR	152	16.587	9.674	37.772	1.00	42.88	B
ATOM	1067	OG1	THR	152	16.143	8.375	37.365	1.00	46.42	B
ATOM	1068	CG2	THR	152	16.182	9.891	39.221	1.00	43.02	B
ATOM	1069	C	THR	152	16.537	12.108	37.216	1.00	42.92	B
ATOM	1070	O	THR	152	17.753	12.303	37.176	1.00	45.15	B
ATOM	1071	N	GLU	153	15.657	13.050	37.539	1.00	41.16	B
ATOM	1072	CA	GLU	153	16.083	14.390	37.910	1.00	39.15	B
ATOM	1073	CB	GLU	153	14.902	15.350	37.865	1.00	41.46	B
ATOM	1074	CG	GLU	153	15.290	16.742	37.456	1.00	46.88	B
ATOM	1075	CD	GLU	153	15.645	16.826	35.983	1.00	50.26	B
ATOM	1076	OE1	GLU	153	16.309	17.808	35.591	1.00	54.28	B
ATOM	1077	OE2	GLU	153	15.256	15.920	35.216	1.00	50.49	B
ATOM	1078	C	GLU	153	16.601	14.273	39.336	1.00	35.77	B
ATOM	1079	O	GLU	153	16.024	13.550	40.143	1.00	34.39	B
ATOM	1080	N	PHE	154	17.676	14.986	39.649	1.00	32.19	B
ATOM	1081	CA	PHE	154	18.247	14.903	40.985	1.00	29.64	B
ATOM	1082	CB	PHE	154	19.221	13.731	41.036	1.00	26.07	B
ATOM	1083	CG	PHE	154	20.478	13.959	40.244	1.00	22.24	B
ATOM	1084	CD1	PHE	154	21.634	14.413	40.870	1.00	19.12	B
ATOM	1085	CD2	PHE	154	20.502	13.725	38.873	1.00	19.79	B
ATOM	1086	CE1	PHE	154	22.804	14.627	40.140	1.00	20.17	B

ATOM	1087	CE2	PHE	154	21.665	13.938	38.132	1.00	19.68	B
ATOM	1088	CZ	PHE	154	22.819	14.388	38.768	1.00	18.22	B
ATOM	1089	C	PHE	154	18.983	16.153	41.462	1.00	28.59	B
ATOM	1090	O	PHE	154	19.343	17.025	40.687	1.00	28.03	B
ATOM	1091	N	SER	155	19.219	16.194	42.765	1.00	28.62	B
ATOM	1092	CA	SER	155	19.940	17.286	43.398	1.00	29.65	B
ATOM	1093	CB	SER	155	18.958	18.297	44.007	1.00	29.30	B
ATOM	1094	OG	SER	155	18.373	17.825	45.210	1.00	30.25	B
ATOM	1095	C	SER	155	20.812	16.670	44.495	1.00	29.32	B
ATOM	1096	O	SER	155	20.364	15.799	45.236	1.00	28.78	B
ATOM	1097	N	VAL	156	22.057	17.117	44.601	1.00	28.25	B
ATOM	1098	CA	VAL	156	22.945	16.571	45.622	1.00	27.65	B
ATOM	1099	CB	VAL	156	24.266	16.059	45.002	1.00	27.82	B
ATOM	1100	CG1	VAL	156	25.067	15.296	46.051	1.00	26.25	B
ATOM	1101	CG2	VAL	156	23.970	15.178	43.793	1.00	26.92	B
ATOM	1102	C	VAL	156	23.293	17.600	46.697	1.00	28.00	B
ATOM	1103	O	VAL	156	23.691	18.705	46.386	1.00	27.61	B
ATOM	1104	N	LYS	157	23.135	17.210	47.961	1.00	28.26	B
ATOM	1105	CA	LYS	157	23.455	18.066	49.107	1.00	29.25	B
ATOM	1106	CB	LYS	157	22.188	18.423	49.897	1.00	30.98	B
ATOM	1107	CG	LYS	157	21.322	19.485	49.261	1.00	34.09	B
ATOM	1108	CD	LYS	157	20.065	19.741	50.080	1.00	37.95	B
ATOM	1109	CE	LYS	157	19.399	21.060	49.665	1.00	41.02	B
ATOM	1110	NZ	LYS	157	20.186	22.277	50.077	1.00	41.43	B
ATOM	1111	C	LYS	157	24.426	17.349	50.047	1.00	28.34	B
ATOM	1112	O	LYS	157	24.195	16.217	50.413	1.00	28.14	B
ATOM	1113	N	VAL	158	25.510	18.016	50.433	1.00	27.07	B
ATOM	1114	CA	VAL	158	26.480	17.412	51.342	1.00	27.48	B
ATOM	1115	CB	VAL	158	27.883	17.280	50.694	1.00	26.91	B
ATOM	1116	CG1	VAL	158	27.811	16.356	49.489	1.00	27.77	B
ATOM	1117	CG2	VAL	158	28.415	18.648	50.301	1.00	27.25	B
ATOM	1118	C	VAL	158	26.629	18.183	52.651	1.00	28.66	B
ATOM	1119	O	VAL	158	26.444	19.393	52.705	1.00	27.69	B
ATOM	1120	N	SER	159	26.973	17.460	53.708	1.00	28.98	B
ATOM	1121	CA	SER	159	27.155	18.058	55.013	1.00	30.95	B
ATOM	1122	CB	SER	159	25.869	17.953	55.823	1.00	32.26	B
ATOM	1123	OG	SER	159	24.817	18.602	55.132	1.00	38.42	B
ATOM	1124	C	SER	159	28.289	17.362	55.736	1.00	30.96	B
ATOM	1125	O	SER	159	28.388	16.146	55.722	1.00	34.27	B
ATOM	1126	N	LEU	160	29.158	18.143	56.357	1.00	29.31	B
ATOM	1127	CA	LEU	160	30.280	17.577	57.064	1.00	27.33	B
ATOM	1128	CB	LEU	160	31.582	18.130	56.499	1.00	27.18	B
ATOM	1129	CG	LEU	160	32.856	17.456	56.991	1.00	28.13	B
ATOM	1130	CD1	LEU	160	32.751	15.954	56.790	1.00	29.56	B
ATOM	1131	CD2	LEU	160	34.044	18.019	56.237	1.00	28.17	B
ATOM	1132	C	LEU	160	30.167	17.884	58.552	1.00	28.09	B
ATOM	1133	O	LEU	160	30.607	18.943	59.026	1.00	26.39	B
ATOM	1134	N	LEU	161	29.558	16.949	59.276	1.00	25.48	B
ATOM	1135	CA	LEU	161	29.371	17.075	60.710	1.00	23.19	B
ATOM	1136	CB	LEU	161	27.982	16.567	61.101	1.00	21.33	B
ATOM	1137	CG	LEU	161	27.694	16.395	62.594	1.00	19.50	B
ATOM	1138	CD1	LEU	161	27.772	17.736	63.288	1.00	19.94	B
ATOM	1139	CD2	LEU	161	26.314	15.775	62.782	1.00	17.88	B
ATOM	1140	C	LEU	161	30.452	16.264	61.415	1.00	23.39	B
ATOM	1141	O	LEU	161	30.641	15.094	61.129	1.00	25.56	B
ATOM	1142	N	GLU	162	31.165	16.899	62.336	1.00	22.32	B
ATOM	1143	CA	GLU	162	32.232	16.237	63.065	1.00	19.98	B
ATOM	1144	CB	GLU	162	33.574	16.839	62.650	1.00	17.28	B
ATOM	1145	CG	GLU	162	33.762	16.859	61.137	1.00	15.11	B
ATOM	1146	CD	GLU	162	35.212	16.937	60.737	1.00	15.23	B
ATOM	1147	OE1	GLU	162	36.063	17.134	61.621	1.00	15.82	B
ATOM	1148	OE2	GLU	162	35.513	16.813	59.539	1.00	17.71	B
ATOM	1149	C	GLU	162	32.031	16.344	64.573	1.00	19.72	B
ATOM	1150	O	GLU	162	31.468	17.299	65.059	1.00	20.94	B
ATOM	1151	N	ILE	163	32.503	15.348	65.312	1.00	18.63	B
ATOM	1152	CA	ILE	163	32.346	15.350	66.756	1.00	18.63	B
ATOM	1153	CB	ILE	163	31.544	14.120	67.223	1.00	19.02	B
ATOM	1154	CG2	ILE	163	31.324	14.178	68.742	1.00	16.34	B
ATOM	1155	CG1	ILE	163	30.210	14.072	66.466	1.00	20.01	B
ATOM	1156	CD1	ILE	163	29.479	12.746	66.563	1.00	22.19	B
ATOM	1157	C	ILE	163	33.694	15.353	67.467	1.00	20.32	B
ATOM	1158	O	ILE	163	34.616	14.672	67.050	1.00	21.59	B
ATOM	1159	N	TYR	164	33.799	16.131	68.542	1.00	20.27	B

ATOM	1160	CA	TYR	164	35.031	16.206	69.312	1.00	19.81	B
ATOM	1161	CB	TYR	164	35.964	17.271	68.709	1.00	20.16	B
ATOM	1162	CG	TYR	164	37.269	17.434	69.451	1.00	17.18	B
ATOM	1163	CD1	TYR	164	37.334	18.191	70.622	1.00	16.03	B
ATOM	1164	CE1	TYR	164	38.506	18.253	71.372	1.00	16.71	B
ATOM	1165	CD2	TYR	164	38.416	16.756	69.042	1.00	18.67	B
ATOM	1166	CE2	TYR	164	39.594	16.812	69.789	1.00	16.74	B
ATOM	1167	CZ	TYR	164	39.627	17.557	70.954	1.00	14.83	B
ATOM	1168	OH	TYR	164	40.758	17.569	71.726	1.00	14.97	B
ATOM	1169	C	TYR	164	34.685	16.520	70.761	1.00	21.32	B
ATOM	1170	O	TYR	164	33.971	17.468	71.044	1.00	22.71	B
ATOM	1171	N	ASN	165	35.185	15.694	71.672	1.00	22.32	B
ATOM	1172	CA	ASN	165	34.926	15.860	73.092	1.00	23.78	B
ATOM	1173	CB	ASN	165	35.722	17.043	73.636	1.00	27.16	B
ATOM	1174	CG	ASN	165	35.729	17.090	75.149	1.00	31.99	B
ATOM	1175	OD1	ASN	165	36.159	16.150	75.801	1.00	37.27	B
ATOM	1176	ND2	ASN	165	35.249	18.190	75.714	1.00	32.43	B
ATOM	1177	C	ASN	165	33.431	16.088	73.313	1.00	24.23	B
ATOM	1178	O	ASN	165	33.034	16.915	74.130	1.00	25.34	B
ATOM	1179	N	GLU	166	32.615	15.340	72.572	1.00	22.37	B
ATOM	1180	CA	GLU	166	31.154	15.421	72.641	1.00	22.51	B
ATOM	1181	CB	GLU	166	30.638	15.047	74.044	1.00	19.36	B
ATOM	1182	CG	GLU	166	30.620	13.540	74.319	1.00	20.22	B
ATOM	1183	CD	GLU	166	29.915	12.746	73.222	1.00	20.01	B
ATOM	1184	OE1	GLU	166	28.668	12.648	73.240	1.00	19.99	B
ATOM	1185	OE2	GLU	166	30.618	12.228	72.330	1.00	16.45	B
ATOM	1186	C	GLU	166	30.570	16.770	72.223	1.00	22.98	B
ATOM	1187	O	GLU	166	29.553	17.189	72.725	1.00	22.40	B
ATOM	1188	N	GLU	167	31.229	17.443	71.288	1.00	25.41	B
ATOM	1189	CA	GLU	167	30.739	18.721	70.793	1.00	27.30	B
ATOM	1190	CB	GLU	167	31.679	19.858	71.191	1.00	29.98	B
ATOM	1191	CG	GLU	167	31.567	20.295	72.648	1.00	34.85	B
ATOM	1192	CD	GLU	167	32.384	21.553	72.941	1.00	39.75	B
ATOM	1193	OE1	GLU	167	33.635	21.487	72.865	1.00	39.56	B
ATOM	1194	OE2	GLU	167	31.771	22.608	73.237	1.00	41.26	B
ATOM	1195	C	GLU	167	30.637	18.626	69.278	1.00	28.54	B
ATOM	1196	O	GLU	167	31.495	18.046	68.633	1.00	29.56	B
ATOM	1197	N	LEU	168	29.574	19.190	68.719	1.00	28.34	B
ATOM	1198	CA	LEU	168	29.367	19.138	67.280	1.00	28.28	B
ATOM	1199	CB	LEU	168	27.865	19.078	66.955	1.00	30.49	B
ATOM	1200	CG	LEU	168	27.009	17.925	67.512	1.00	30.82	B
ATOM	1201	CD1	LEU	168	27.623	16.583	67.142	1.00	31.07	B
ATOM	1202	CD2	LEU	168	26.892	18.044	69.009	1.00	33.15	B
ATOM	1203	C	LEU	168	29.997	20.322	66.563	1.00	26.93	B
ATOM	1204	O	LEU	168	29.972	21.442	67.064	1.00	28.48	B
ATOM	1205	N	PHE	169	30.562	20.069	65.386	1.00	24.01	B
ATOM	1206	CA	PHE	169	31.191	21.112	64.584	1.00	22.58	B
ATOM	1207	CB	PHE	169	32.723	21.073	64.727	1.00	22.71	B
ATOM	1208	CG	PHE	169	33.213	21.377	66.118	1.00	21.76	B
ATOM	1209	CD1	PHE	169	33.451	20.354	67.027	1.00	21.14	B
ATOM	1210	CD2	PHE	169	33.393	22.699	66.534	1.00	22.60	B
ATOM	1211	CE1	PHE	169	33.861	20.628	68.323	1.00	22.05	B
ATOM	1212	CE2	PHE	169	33.802	22.989	67.830	1.00	21.62	B
ATOM	1213	CZ	PHE	169	34.037	21.952	68.729	1.00	24.67	B
ATOM	1214	C	PHE	169	30.824	20.950	63.111	1.00	23.10	B
ATOM	1215	O	PHE	169	30.612	19.836	62.634	1.00	20.06	B
ATOM	1216	N	ASP	170	30.739	22.079	62.406	1.00	22.96	B
ATOM	1217	CA	ASP	170	30.416	22.100	60.978	1.00	22.20	B
ATOM	1218	CB	ASP	170	29.344	23.148	60.679	1.00	20.54	B
ATOM	1219	CG	ASP	170	28.799	23.048	59.257	1.00	21.66	B
ATOM	1220	OD1	ASP	170	29.554	22.671	58.337	1.00	18.77	B
ATOM	1221	OD2	ASP	170	27.602	23.358	59.065	1.00	23.66	B
ATOM	1222	C	ASP	170	31.680	22.466	60.211	1.00	22.85	B
ATOM	1223	O	ASP	170	32.108	23.621	60.242	1.00	25.36	B
ATOM	1224	N	LEU	171	32.280	21.490	59.529	1.00	22.35	B
ATOM	1225	CA	LEU	171	33.494	21.729	58.764	1.00	22.58	B
ATOM	1226	CB	LEU	171	34.430	20.533	58.864	1.00	16.27	B
ATOM	1227	CG	LEU	171	35.235	20.424	60.169	1.00	16.39	B
ATOM	1228	CD1	LEU	171	36.234	21.577	60.274	1.00	14.32	B
ATOM	1229	CD2	LEU	171	34.304	20.421	61.351	1.00	12.71	B
ATOM	1230	C	LEU	171	33.257	22.082	57.300	1.00	26.58	B
ATOM	1231	O	LEU	171	34.167	21.976	56.479	1.00	26.75	B
ATOM	1232	N	LEU	172	32.038	22.510	56.978	1.00	29.45	B

ATOM	1233	CA	LEU	172	31.706	22.898	55.612	1.00	34.57	B
ATOM	1234	CB	LEU	172	30.742	21.892	54.975	1.00	33.36	B
ATOM	1235	CG	LEU	172	31.387	20.715	54.244	1.00	31.35	B
ATOM	1236	CD1	LEU	172	30.316	19.992	53.459	1.00	32.85	B
ATOM	1237	CD2	LEU	172	32.473	21.201	53.302	1.00	32.08	B
ATOM	1238	C	LEU	172	31.107	24.297	55.531	1.00	38.00	B
ATOM	1239	O	LEU	172	30.961	24.850	54.457	1.00	39.59	B
ATOM	1240	N	ASN	173	30.766	24.865	56.679	1.00	41.36	B
ATOM	1241	CA	ASN	173	30.201	26.205	56.714	1.00	45.99	B
ATOM	1242	CB	ASN	173	29.401	26.405	58.003	1.00	47.65	B
ATOM	1243	CG	ASN	173	28.670	27.735	58.038	1.00	50.77	B
ATOM	1244	OD1	ASN	173	28.005	28.060	59.014	1.00	51.85	B
ATOM	1245	ND2	ASN	173	28.792	28.508	56.964	1.00	51.20	B
ATOM	1246	C	ASN	173	31.346	27.214	56.643	1.00	48.84	B
ATOM	1247	O	ASN	173	32.070	27.403	57.606	1.00	48.46	B
ATOM	1248	N	PRO	174	31.521	27.872	55.484	1.00	52.47	B
ATOM	1249	CD	PRO	174	30.710	27.738	54.258	1.00	53.23	B
ATOM	1250	CA	PRO	174	32.587	28.862	55.289	1.00	55.00	B
ATOM	1251	CB	PRO	174	32.542	29.116	53.786	1.00	53.92	B
ATOM	1252	CG	PRO	174	31.089	28.983	53.482	1.00	52.93	B
ATOM	1253	C	PRO	174	32.396	30.141	56.095	1.00	58.07	B
ATOM	1254	O	PRO	174	33.329	30.921	56.263	1.00	58.84	B
ATOM	1255	N	SER	175	31.183	30.343	56.596	1.00	60.39	B
ATOM	1256	CA	SER	175	30.861	31.534	57.372	1.00	62.65	B
ATOM	1257	CB	SER	175	29.343	31.666	57.498	1.00	63.30	B
ATOM	1258	OG	SER	175	28.723	31.545	56.230	1.00	65.14	B
ATOM	1259	C	SER	175	31.500	31.535	58.759	1.00	63.89	B
ATOM	1260	O	SER	175	32.365	32.358	59.051	1.00	65.71	B
ATOM	1261	N	SER	176	31.066	30.608	59.608	1.00	64.41	B
ATOM	1262	CA	SER	176	31.581	30.506	60.969	1.00	64.51	B
ATOM	1263	CB	SER	176	30.597	29.725	61.844	1.00	64.33	B
ATOM	1264	OG	SER	176	30.446	28.396	61.378	1.00	64.08	B
ATOM	1265	C	SER	176	32.942	29.824	61.012	1.00	64.78	B
ATOM	1266	O	SER	176	33.474	29.418	59.984	1.00	64.25	B
ATOM	1267	N	ASP	177	33.500	29.704	62.213	1.00	65.17	B
ATOM	1268	CA	ASP	177	34.789	29.051	62.379	1.00	65.62	B
ATOM	1269	CB	ASP	177	35.782	29.964	63.106	1.00	66.73	B
ATOM	1270	CG	ASP	177	35.449	30.137	64.576	1.00	68.48	B
ATOM	1271	OD1	ASP	177	36.388	30.344	65.377	1.00	67.76	B
ATOM	1272	OD2	ASP	177	34.251	30.069	64.929	1.00	69.81	B
ATOM	1273	C	ASP	177	34.615	27.757	63.166	1.00	64.60	B
ATOM	1274	O	ASP	177	33.498	27.335	63.445	1.00	64.22	B
ATOM	1275	N	VAL	178	35.737	27.146	63.529	1.00	63.40	B
ATOM	1276	CA	VAL	178	35.735	25.890	64.264	1.00	62.69	B
ATOM	1277	CB	VAL	178	37.046	25.116	64.016	1.00	62.85	B
ATOM	1278	CG1	VAL	178	37.190	24.809	62.536	1.00	61.71	B
ATOM	1279	CG2	VAL	178	38.231	25.934	64.510	1.00	62.99	B
ATOM	1280	C	VAL	178	35.552	26.050	65.770	1.00	61.94	B
ATOM	1281	O	VAL	178	35.792	25.122	66.524	1.00	62.60	B
ATOM	1282	N	SER	179	35.124	27.227	66.208	1.00	61.07	B
ATOM	1283	CA	SER	179	34.922	27.447	67.632	1.00	59.46	B
ATOM	1284	CB	SER	179	35.629	28.731	68.080	1.00	59.42	B
ATOM	1285	OG	SER	179	35.030	29.877	67.507	1.00	59.13	B
ATOM	1286	C	SER	179	33.437	27.517	67.977	1.00	58.68	B
ATOM	1287	O	SER	179	33.067	27.489	69.144	1.00	59.17	B
ATOM	1288	N	GLU	180	32.591	27.605	66.955	1.00	56.65	B
ATOM	1289	CA	GLU	180	31.145	27.671	67.161	1.00	55.22	B
ATOM	1290	CB	GLU	180	30.507	28.607	66.129	1.00	56.66	B
ATOM	1291	CG	GLU	180	30.550	30.079	66.535	1.00	59.12	B
ATOM	1292	CD	GLU	180	30.230	31.032	65.392	1.00	60.03	B
ATOM	1293	OE1	GLU	180	31.066	31.163	64.474	1.00	60.45	B
ATOM	1294	OE2	GLU	180	29.143	31.650	65.411	1.00	61.47	B
ATOM	1295	C	GLU	180	30.498	26.293	67.080	1.00	52.95	B
ATOM	1296	O	GLU	180	30.207	25.803	66.004	1.00	52.86	B
ATOM	1297	N	ARG	181	30.285	25.679	68.239	1.00	51.12	B
ATOM	1298	CA	ARG	181	29.675	24.360	68.315	1.00	48.73	B
ATOM	1299	CB	ARG	181	29.835	23.793	69.727	1.00	51.62	B
ATOM	1300	CG	ARG	181	29.642	24.816	70.836	1.00	56.45	B
ATOM	1301	CD	ARG	181	28.829	24.256	72.007	1.00	61.65	B
ATOM	1302	NE	ARG	181	27.400	24.135	71.702	1.00	64.33	B
ATOM	1303	CZ	ARG	181	26.483	23.692	72.560	1.00	65.71	B
ATOM	1304	NH1	ARG	181	26.834	23.324	73.786	1.00	66.05	B
ATOM	1305	NH2	ARG	181	25.209	23.616	72.194	1.00	66.36	B

ATOM	1306	C	ARG	181	28.196	24.403	67.940	1.00	45.46		B
ATOM	1307	O	ARG	181	27.556	25.438	68.029	1.00	45.33		B
ATOM	1308	N	LEU	182	27.661	23.267	67.510	1.00	41.98		B
ATOM	1309	CA	LEU	182	26.258	23.193	67.133	1.00	38.04		B
ATOM	1310	CB	LEU	182	26.099	22.419	65.824	1.00	35.02		B
ATOM	1311	CG	LEU	182	26.990	22.896	64.677	1.00	33.00		B
ATOM	1312	CD1	LEU	182	26.723	22.060	63.450	1.00	31.57		B
ATOM	1313	CD2	LEU	182	26.733	24.372	64.393	1.00	32.49		B
ATOM	1314	C	LEU	182	25.456	22.524	68.236	1.00	38.00		B
ATOM	1315	O	LEU	182	26.017	21.845	69.096	1.00	37.75		B
ATOM	1316	N	GLN	183	24.140	22.723	68.206	1.00	37.43		B
ATOM	1317	CA	GLN	183	23.239	22.148	69.200	1.00	36.96		B
ATOM	1318	CB	GLN	183	22.269	23.210	69.724	1.00	38.87		B
ATOM	1319	CG	GLN	183	22.925	24.543	70.024	1.00	43.04		B
ATOM	1320	CD	GLN	183	21.969	25.536	70.653	1.00	45.13		B
ATOM	1321	OE1	GLN	183	21.663	25.448	71.832	1.00	45.23		B
ATOM	1322	NE2	GLN	183	21.493	26.492	69.856	1.00	46.40		B
ATOM	1323	C	GLN	183	22.455	21.018	68.567	1.00	35.80		B
ATOM	1324	O	GLN	183	22.097	21.073	67.397	1.00	33.40		B
ATOM	1325	N	MET	184	22.165	20.005	69.367	1.00	36.43		B
ATOM	1326	CA	MET	184	21.450	18.840	68.877	1.00	37.65		B
ATOM	1327	CB	MET	184	22.322	17.610	69.118	1.00	38.53		B
ATOM	1328	CG	MET	184	22.033	16.445	68.221	1.00	41.45		B
ATOM	1329	SD	MET	184	23.141	15.085	68.586	1.00	42.59		B
ATOM	1330	CE	MET	184	22.590	14.660	70.190	1.00	40.16		B
ATOM	1331	C	MET	184	20.111	18.692	69.590	1.00	37.82		B
ATOM	1332	O	MET	184	20.021	18.909	70.790	1.00	37.22		B
ATOM	1333	N	PHE	185	19.070	18.328	68.844	1.00	39.01		B
ATOM	1334	CA	PHE	185	17.741	18.148	69.432	1.00	41.26		B
ATOM	1335	CB	PHE	185	16.851	19.377	69.160	1.00	40.10		B
ATOM	1336	CG	PHE	185	17.499	20.697	69.494	1.00	38.50		B
ATOM	1337	CD1	PHE	185	18.249	21.377	68.544	1.00	36.52		B
ATOM	1338	CD2	PHE	185	17.376	21.248	70.770	1.00	38.29		B
ATOM	1339	CE1	PHE	185	18.869	22.586	68.851	1.00	37.06		B
ATOM	1340	CE2	PHE	185	17.994	22.459	71.089	1.00	37.60		B
ATOM	1341	CZ	PHE	185	18.743	23.128	70.128	1.00	37.41		B
ATOM	1342	C	PHE	185	17.034	16.903	68.887	1.00	43.21		B
ATOM	1343	O	PHE	185	17.221	16.532	67.734	1.00	41.62		B
ATOM	1344	N	ASP	186	16.223	16.259	69.724	1.00	46.68		B
ATOM	1345	CA	ASP	186	15.482	15.078	69.286	1.00	51.00		B
ATOM	1346	CB	ASP	186	14.722	14.437	70.449	1.00	52.32		B
ATOM	1347	CG	ASP	186	15.642	13.912	71.530	1.00	54.63		B
ATOM	1348	OD1	ASP	186	16.575	13.150	71.202	1.00	55.59		B
ATOM	1349	OD2	ASP	186	15.428	14.262	72.712	1.00	56.98		B
ATOM	1350	C	ASP	186	14.481	15.539	68.241	1.00	52.48		B
ATOM	1351	O	ASP	186	13.777	16.510	68.443	1.00	52.99		B
ATOM	1352	N	ASP	187	14.425	14.841	67.118	1.00	55.70		B
ATOM	1353	CA	ASP	187	13.500	15.214	66.061	1.00	59.24		B
ATOM	1354	CB	ASP	187	13.845	14.469	64.772	1.00	58.33		B
ATOM	1355	CG	ASP	187	13.015	14.929	63.601	1.00	58.32		B
ATOM	1356	OD1	ASP	187	13.345	14.546	62.459	1.00	59.29		B
ATOM	1357	OD2	ASP	187	12.035	15.672	63.822	1.00	58.82		B
ATOM	1358	C	ASP	187	12.064	14.905	66.473	1.00	61.85		B
ATOM	1359	O	ASP	187	11.690	13.750	66.626	1.00	62.59		B
ATOM	1360	N	PRO	188	11.241	15.950	66.662	1.00	64.18		B
ATOM	1361	CD	PRO	188	11.573	17.374	66.493	1.00	64.61		B
ATOM	1362	CA	PRO	188	9.840	15.794	67.061	1.00	66.06		B
ATOM	1363	CB	PRO	188	9.287	17.207	66.923	1.00	65.95		B
ATOM	1364	CG	PRO	188	10.472	18.048	67.271	1.00	65.81		B
ATOM	1365	C	PRO	188	9.094	14.793	66.189	1.00	68.16		B
ATOM	1366	O	PRO	188	8.316	13.981	66.687	1.00	67.45		B
ATOM	1367	N	ARG	189	9.345	14.854	64.886	1.00	70.27		B
ATOM	1368	CA	ARG	189	8.702	13.949	63.944	1.00	73.47		B
ATOM	1369	CB	ARG	189	9.278	14.170	62.547	1.00	73.94		B
ATOM	1370	CG	ARG	189	8.869	15.498	61.926	1.00	75.92		B
ATOM	1371	CD	ARG	189	9.507	15.693	60.558	1.00	77.54		B
ATOM	1372	NE	ARG	189	10.797	16.373	60.644	1.00	78.29		B
ATOM	1373	CZ	ARG	189	10.940	17.686	60.804	1.00	78.57		B
ATOM	1374	NH1	ARG	189	9.870	18.466	60.894	1.00	78.77		B
ATOM	1375	NH2	ARG	189	12.153	18.218	60.873	1.00	78.05		B
ATOM	1376	C	ARG	189	8.869	12.491	64.363	1.00	75.30		B
ATOM	1377	O	ARG	189	7.896	11.815	64.683	1.00	75.56		B
ATOM	1378	N	ASN	190	10.112	12.019	64.370	1.00	77.42		B

ATOM	1379	CA	ASN	190	10.417	10.640	64.748	1.00	78.69	B
ATOM	1380	CB	ASN	190	10.760	9.829	63.494	1.00	78.94	B
ATOM	1381	CG	ASN	190	11.569	10.629	62.483	1.00	78.61	B
ATOM	1382	OD1	ASN	190	12.745	10.905	62.689	1.00	78.52	B
ATOM	1383	ND2	ASN	190	10.926	11.011	61.383	1.00	78.16	B
ATOM	1384	C	ASN	190	11.571	10.575	65.749	1.00	79.40	B
ATOM	1385	O	ASN	190	12.706	10.875	65.408	1.00	79.98	B
ATOM	1386	N	LYS	191	11.265	10.182	66.986	1.00	79.97	B
ATOM	1387	CA	LYS	191	12.267	10.084	68.051	1.00	79.77	B
ATOM	1388	CB	LYS	191	11.616	9.561	69.336	1.00	81.11	B
ATOM	1389	CG	LYS	191	10.794	10.600	70.090	1.00	82.60	B
ATOM	1390	CD	LYS	191	11.695	11.630	70.758	1.00	83.37	B
ATOM	1391	CE	LYS	191	10.887	12.716	71.450	1.00	84.12	B
ATOM	1392	NZ	LYS	191	10.109	13.539	70.478	1.00	84.72	B
ATOM	1393	C	LYS	191	13.478	9.216	67.695	1.00	78.46	B
ATOM	1394	O	LYS	191	14.462	9.173	68.434	1.00	77.59	B
ATOM	1395	N	ARG	192	13.398	8.525	66.563	1.00	76.93	B
ATOM	1396	CA	ARG	192	14.489	7.675	66.106	1.00	75.17	B
ATOM	1397	CB	ARG	192	13.975	6.667	65.078	1.00	77.95	B
ATOM	1398	CG	ARG	192	15.041	5.708	64.573	1.00	80.81	B
ATOM	1399	CD	ARG	192	14.801	5.305	63.122	1.00	83.98	B
ATOM	1400	NE	ARG	192	14.928	6.434	62.198	1.00	86.03	B
ATOM	1401	CZ	ARG	192	13.946	7.277	61.884	1.00	86.70	B
ATOM	1402	NH1	ARG	192	12.737	7.133	62.415	1.00	86.57	B
ATOM	1403	NH2	ARG	192	14.175	8.267	61.033	1.00	87.03	B
ATOM	1404	C	ARG	192	15.565	8.545	65.463	1.00	72.66	B
ATOM	1405	O	ARG	192	16.699	8.112	65.272	1.00	72.31	B
ATOM	1406	N	GLY	193	15.195	9.781	65.136	1.00	69.32	B
ATOM	1407	CA	GLY	193	16.132	10.695	64.507	1.00	63.90	B
ATOM	1408	C	GLY	193	16.538	11.863	65.382	1.00	59.50	B
ATOM	1409	O	GLY	193	16.132	11.961	66.531	1.00	59.54	B
ATOM	1410	N	VAL	194	17.346	12.757	64.824	1.00	55.13	B
ATOM	1411	CA	VAL	194	17.812	13.918	65.562	1.00	50.91	B
ATOM	1412	CB	VAL	194	19.114	13.606	66.309	1.00	50.28	B
ATOM	1413	CG1	VAL	194	20.226	13.319	65.318	1.00	49.18	B
ATOM	1414	CG2	VAL	194	19.476	14.760	67.207	1.00	48.67	B
ATOM	1415	C	VAL	194	18.055	15.098	64.629	1.00	49.13	B
ATOM	1416	O	VAL	194	18.379	14.918	63.461	1.00	49.22	B
ATOM	1417	N	ILE	195	17.906	16.308	65.160	1.00	46.55	B
ATOM	1418	CA	ILE	195	18.106	17.514	64.372	1.00	42.49	B
ATOM	1419	CB	ILE	195	16.846	18.405	64.396	1.00	43.57	B
ATOM	1420	CG2	ILE	195	17.076	19.653	63.561	1.00	44.86	B
ATOM	1421	CG1	ILE	195	15.647	17.639	63.837	1.00	44.25	B
ATOM	1422	CD1	ILE	195	15.828	17.184	62.393	1.00	45.64	B
ATOM	1423	C	ILE	195	19.291	18.349	64.856	1.00	39.72	B
ATOM	1424	O	ILE	195	19.379	18.691	66.030	1.00	38.69	B
ATOM	1425	N	ILE	196	20.197	18.672	63.936	1.00	37.40	B
ATOM	1426	CA	ILE	196	21.365	19.483	64.255	1.00	35.21	B
ATOM	1427	CB	ILE	196	22.654	18.960	63.561	1.00	34.42	B
ATOM	1428	CG2	ILE	196	23.821	19.880	63.881	1.00	33.62	B
ATOM	1429	CG1	ILE	196	23.010	17.552	64.057	1.00	33.50	B
ATOM	1430	CD1	ILE	196	22.222	16.445	63.416	1.00	31.23	B
ATOM	1431	C	ILE	196	21.113	20.920	63.806	1.00	35.34	B
ATOM	1432	O	ILE	196	21.108	21.218	62.619	1.00	33.58	B
ATOM	1433	N	LYS	197	20.912	21.806	64.777	1.00	36.02	B
ATOM	1434	CA	LYS	197	20.639	23.209	64.494	1.00	36.95	B
ATOM	1435	CB	LYS	197	20.101	23.909	65.744	1.00	37.83	B
ATOM	1436	CG	LYS	197	19.736	25.370	65.519	1.00	42.01	B
ATOM	1437	CD	LYS	197	19.391	26.055	66.829	1.00	45.50	B
ATOM	1438	CE	LYS	197	19.039	27.518	66.628	1.00	46.65	B
ATOM	1439	NZ	LYS	197	18.686	28.161	67.932	1.00	47.32	B
ATOM	1440	C	LYS	197	21.857	23.968	63.983	1.00	36.01	B
ATOM	1441	O	LYS	197	22.887	24.025	64.646	1.00	34.47	B
ATOM	1442	N	GLY	198	21.722	24.547	62.793	1.00	35.82	B
ATOM	1443	CA	GLY	198	22.809	25.316	62.212	1.00	37.33	B
ATOM	1444	C	GLY	198	23.715	24.583	61.240	1.00	38.13	B
ATOM	1445	O	GLY	198	24.580	25.198	60.615	1.00	39.69	B
ATOM	1446	N	LEU	199	23.530	23.275	61.098	1.00	37.34	B
ATOM	1447	CA	LEU	199	24.376	22.512	60.190	1.00	36.62	B
ATOM	1448	CB	LEU	199	24.218	21.006	60.444	1.00	34.70	B
ATOM	1449	CG	LEU	199	25.067	20.058	59.588	1.00	33.44	B
ATOM	1450	CD1	LEU	199	26.553	20.355	59.755	1.00	31.11	B
ATOM	1451	CD2	LEU	199	24.767	18.634	59.994	1.00	32.49	B

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ATOM   1452  C   LEU  199      24.066  22.838  58.729  1.00 36.33      B
ATOM   1453  O   LEU  199      22.971  22.550  58.228  1.00 35.86      B
ATOM   1454  N   GLU  200      25.040  23.441  58.053  1.00 35.51      B
ATOM   1455  CA  GLU  200      24.896  23.815  56.653  1.00 37.46      B
ATOM   1456  CB  GLU  200      26.037  24.746  56.234  1.00 40.69      B
ATOM   1457  CG  GLU  200      26.005  26.135  56.868  1.00 49.20      B
ATOM   1458  CD  GLU  200      24.757  26.925  56.502  1.00 51.96      B
ATOM   1459  OE1 GLU  200      23.659  26.576  56.990  1.00 54.11      B
ATOM   1460  OE2 GLU  200      24.873  27.896  55.722  1.00 54.04      B
ATOM   1461  C   GLU  200      24.874  22.612  55.717  1.00 36.14      B
ATOM   1462  O   GLU  200      25.434  21.564  56.015  1.00 35.01      B
ATOM   1463  N   GLU  201      24.217  22.787  54.575  1.00 35.47      B
ATOM   1464  CA  GLU  201      24.124  21.752  53.559  1.00 34.36      B
ATOM   1465  CB  GLU  201      22.709  21.189  53.483  1.00 34.40      B
ATOM   1466  CG  GLU  201      22.207  20.582  54.773  1.00 34.93      B
ATOM   1467  CD  GLU  201      20.816  19.998  54.626  1.00 36.86      B
ATOM   1468  OE1 GLU  201      20.137  19.825  55.665  1.00 37.44      B
ATOM   1469  OE2 GLU  201      20.408  19.710  53.476  1.00 36.10      B
ATOM   1470  C   GLU  201      24.479  22.393  52.226  1.00 34.09      B
ATOM   1471  O   GLU  201      23.681  23.115  51.657  1.00 33.70      B
ATOM   1472  N   ILE  202      25.687  22.127  51.740  1.00 33.17      B
ATOM   1473  CA  ILE  202      26.130  22.689  50.472  1.00 32.42      B
ATOM   1474  CB  ILE  202      27.679  22.715  50.357  1.00 33.25      B
ATOM   1475  CG2 ILE  202      28.087  23.275  49.002  1.00 31.31      B
ATOM   1476  CG1 ILE  202      28.286  23.582  51.465  1.00 33.81      B
ATOM   1477  CD1 ILE  202      28.222  22.967  52.849  1.00 36.54      B
ATOM   1478  C   ILE  202      25.572  21.888  49.305  1.00 31.15      B
ATOM   1479  O   ILE  202      25.703  20.678  49.257  1.00 33.14      B
ATOM   1480  N   THR  203      24.948  22.583  48.361  1.00 29.99      B
ATOM   1481  CA  THR  203      24.371  21.944  47.185  1.00 27.86      B
ATOM   1482  CB  THR  203      23.228  22.804  46.572  1.00 27.52      B
ATOM   1483  OG1 THR  203      22.157  22.925  47.516  1.00 27.78      B
ATOM   1484  CG2 THR  203      22.701  22.174  45.284  1.00 26.79      B
ATOM   1485  C   THR  203      25.448  21.741  46.130  1.00 27.11      B
ATOM   1486  O   THR  203      26.217  22.637  45.853  1.00 26.94      B
ATOM   1487  N   VAL  204      25.500  20.541  45.560  1.00 27.55      B
ATOM   1488  CA  VAL  204      26.467  20.222  44.517  1.00 27.42      B
ATOM   1489  CB  VAL  204      27.136  18.859  44.781  1.00 25.01      B
ATOM   1490  CG1 VAL  204      28.393  18.718  43.941  1.00 23.11      B
ATOM   1491  CG2 VAL  204      27.468  18.729  46.250  1.00 23.76      B
ATOM   1492  C   VAL  204      25.677  20.178  43.207  1.00 29.81      B
ATOM   1493  O   VAL  204      24.887  19.261  42.983  1.00 30.56      B
ATOM   1494  N   HIS  205      25.891  21.188  42.364  1.00 30.97      B
ATOM   1495  CA  HIS  205      25.197  21.318  41.079  1.00 33.24      B
ATOM   1496  CB  HIS  205      25.199  22.792  40.649  1.00 33.42      B
ATOM   1497  CG  HIS  205      24.641  23.716  41.687  1.00 34.00      B
ATOM   1498  CD2 HIS  205      25.233  24.333  42.739  1.00 33.05      B
ATOM   1499  ND1 HIS  205      23.297  24.019  41.771  1.00 33.23      B
ATOM   1500  CE1 HIS  205      23.086  24.777  42.832  1.00 33.03      B
ATOM   1501  NE2 HIS  205      24.244  24.981  43.437  1.00 32.48      B
ATOM   1502  C   HIS  205      25.790  20.450  39.969  1.00 33.72      B
ATOM   1503  O   HIS  205      25.084  20.022  39.061  1.00 32.22      B
ATOM   1504  N   ASN  206      27.094  20.201  40.048  1.00 35.23      B
ATOM   1505  CA  ASN  206      27.779  19.381  39.055  1.00 36.89      B
ATOM   1506  CB  ASN  206      28.178  20.229  37.837  1.00 37.95      B
ATOM   1507  CG  ASN  206      28.999  21.455  38.213  1.00 41.34      B
ATOM   1508  OD1 ASN  206      30.130  21.339  38.697  1.00 43.10      B
ATOM   1509  ND2 ASN  206      28.428  22.641  37.993  1.00 38.53      B
ATOM   1510  C   ASN  206      29.007  18.712  39.666  1.00 36.43      B
ATOM   1511  O   ASN  206      29.233  18.805  40.864  1.00 36.95      B
ATOM   1512  N   LYS  207      29.787  18.029  38.834  1.00 36.70      B
ATOM   1513  CA  LYS  207      30.983  17.338  39.297  1.00 37.65      B
ATOM   1514  CB  LYS  207      31.357  16.232  38.314  1.00 38.65      B
ATOM   1515  CG  LYS  207      31.892  16.726  36.977  1.00 41.42      B
ATOM   1516  CD  LYS  207      31.938  15.585  35.966  1.00 45.62      B
ATOM   1517  CE  LYS  207      32.889  15.877  34.814  1.00 47.44      B
ATOM   1518  NZ  LYS  207      34.314  15.937  35.262  1.00 47.37      B
ATOM   1519  C   LYS  207      32.155  18.298  39.464  1.00 38.02      B
ATOM   1520  O   LYS  207      32.990  18.121  40.340  1.00 38.46      B
ATOM   1521  N   ASP  208      32.199  19.320  38.618  1.00 38.91      B
ATOM   1522  CA  ASP  208      33.264  20.313  38.667  1.00 40.47      B
ATOM   1523  CB  ASP  208      33.316  21.061  37.338  1.00 42.51      B
ATOM   1524  CG  ASP  208      33.664  20.156  36.192  1.00 44.26      B
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ATOM	1525	OD1	ASP	208	33.297	20.470	35.041	1.00	44.33	B
ATOM	1526	OD2	ASP	208	34.321	19.127	36.451	1.00	46.27	B
ATOM	1527	C	ASP	208	33.058	21.300	39.805	1.00	39.34	B
ATOM	1528	O	ASP	208	33.568	22.405	39.780	1.00	40.79	B
ATOM	1529	N	GLU	209	32.308	20.893	40.813	1.00	38.81	B
ATOM	1530	CA	GLU	209	32.050	21.772	41.930	1.00	38.33	B
ATOM	1531	CB	GLU	209	30.604	22.260	41.866	1.00	39.47	B
ATOM	1532	CG	GLU	209	30.278	23.400	42.805	1.00	42.87	B
ATOM	1533	CD	GLU	209	28.824	23.836	42.700	1.00	44.43	B
ATOM	1534	OE1	GLU	209	28.373	24.134	41.573	1.00	42.49	B
ATOM	1535	OE2	GLU	209	28.135	23.885	43.749	1.00	44.53	B
ATOM	1536	C	GLU	209	32.303	21.055	43.247	1.00	37.83	B
ATOM	1537	O	GLU	209	32.147	21.649	44.316	1.00	38.61	B
ATOM	1538	N	VAL	210	32.720	19.790	43.171	1.00	35.54	B
ATOM	1539	CA	VAL	210	32.954	19.011	44.384	1.00	32.37	B
ATOM	1540	CB	VAL	210	32.679	17.485	44.158	1.00	31.94	B
ATOM	1541	CG1	VAL	210	31.641	17.286	43.057	1.00	31.12	B
ATOM	1542	CG2	VAL	210	33.961	16.749	43.842	1.00	30.76	B
ATOM	1543	C	VAL	210	34.342	19.173	44.991	1.00	29.97	B
ATOM	1544	O	VAL	210	34.482	19.206	46.207	1.00	29.98	B
ATOM	1545	N	TYR	211	35.367	19.285	44.154	1.00	27.29	B
ATOM	1546	CA	TYR	211	36.718	19.408	44.685	1.00	25.19	B
ATOM	1547	CB	TYR	211	37.747	19.437	43.549	1.00	24.73	B
ATOM	1548	CG	TYR	211	39.177	19.352	44.040	1.00	26.20	B
ATOM	1549	CD1	TYR	211	39.601	18.278	44.824	1.00	27.98	B
ATOM	1550	CE1	TYR	211	40.903	18.214	45.325	1.00	27.65	B
ATOM	1551	CD2	TYR	211	40.093	20.360	43.761	1.00	26.06	B
ATOM	1552	CE2	TYR	211	41.398	20.308	44.257	1.00	26.72	B
ATOM	1553	CZ	TYR	211	41.797	19.233	45.041	1.00	29.28	B
ATOM	1554	OH	TYR	211	43.081	19.193	45.556	1.00	27.76	B
ATOM	1555	C	TYR	211	36.864	20.635	45.573	1.00	24.67	B
ATOM	1556	O	TYR	211	37.515	20.578	46.615	1.00	24.02	B
ATOM	1557	N	GLN	212	36.251	21.742	45.160	1.00	25.05	B
ATOM	1558	CA	GLN	212	36.294	22.982	45.926	1.00	24.24	B
ATOM	1559	CB	GLN	212	35.508	24.082	45.224	1.00	27.89	B
ATOM	1560	CG	GLN	212	36.375	25.051	44.459	1.00	36.14	B
ATOM	1561	CD	GLN	212	35.625	26.311	44.048	1.00	40.99	B
ATOM	1562	OE1	GLN	212	34.641	26.248	43.312	1.00	42.51	B
ATOM	1563	NE2	GLN	212	36.090	27.465	44.532	1.00	41.52	B
ATOM	1564	C	GLN	212	35.713	22.777	47.305	1.00	22.91	B
ATOM	1565	O	GLN	212	36.285	23.206	48.299	1.00	23.35	B
ATOM	1566	N	ILE	213	34.560	22.122	47.362	1.00	22.44	B
ATOM	1567	CA	ILE	213	33.905	21.876	48.640	1.00	22.31	B
ATOM	1568	CB	ILE	213	32.595	21.095	48.472	1.00	20.76	B
ATOM	1569	CG2	ILE	213	31.910	20.947	49.828	1.00	21.01	B
ATOM	1570	CG1	ILE	213	31.675	21.821	47.492	1.00	20.79	B
ATOM	1571	CD1	ILE	213	30.457	21.012	47.071	1.00	22.47	B
ATOM	1572	C	ILE	213	34.816	21.095	49.573	1.00	22.67	B
ATOM	1573	O	ILE	213	34.863	21.366	50.764	1.00	23.38	B
ATOM	1574	N	LEU	214	35.539	20.126	49.020	1.00	24.93	B
ATOM	1575	CA	LEU	214	36.455	19.307	49.811	1.00	26.22	B
ATOM	1576	CB	LEU	214	36.965	18.129	48.972	1.00	27.09	B
ATOM	1577	CG	LEU	214	36.092	16.868	48.882	1.00	29.34	B
ATOM	1578	CD1	LEU	214	34.618	17.235	48.836	1.00	30.24	B
ATOM	1579	CD2	LEU	214	36.491	16.059	47.649	1.00	30.55	B
ATOM	1580	C	LEU	214	37.621	20.149	50.314	1.00	26.01	B
ATOM	1581	O	LEU	214	38.064	19.994	51.444	1.00	26.33	B
ATOM	1582	N	GLU	215	38.108	21.049	49.464	1.00	25.83	B
ATOM	1583	CA	GLU	215	39.215	21.930	49.834	1.00	24.69	B
ATOM	1584	CB	GLU	215	39.586	22.830	48.655	1.00	23.60	B
ATOM	1585	CG	GLU	215	40.814	22.380	47.882	1.00	22.50	B
ATOM	1586	CD	GLU	215	40.907	23.030	46.511	1.00	23.11	B
ATOM	1587	OE1	GLU	215	42.047	23.251	46.040	1.00	20.98	B
ATOM	1588	OE2	GLU	215	39.839	23.306	45.913	1.00	20.38	B
ATOM	1589	C	GLU	215	38.837	22.784	51.040	1.00	23.82	B
ATOM	1590	O	GLU	215	39.636	22.960	51.967	1.00	23.91	B
ATOM	1591	N	LYS	216	37.617	23.306	51.033	1.00	22.14	B
ATOM	1592	CA	LYS	216	37.152	24.135	52.129	1.00	24.81	B
ATOM	1593	CB	LYS	216	35.794	24.747	51.781	1.00	28.88	B
ATOM	1594	CG	LYS	216	35.875	25.760	50.637	1.00	35.31	B
ATOM	1595	CD	LYS	216	34.492	26.263	50.229	1.00	40.73	B
ATOM	1596	CE	LYS	216	34.591	27.386	49.208	1.00	42.22	B
ATOM	1597	NZ	LYS	216	35.405	27.007	48.007	1.00	44.86	B

ATOM	1598	C	LYS	216	37.066	23.327	53.417	1.00	24.49	B
ATOM	1599	O	LYS	216	37.497	23.790	54.475	1.00	25.43	B
ATOM	1600	N	GLY	217	36.525	22.117	53.325	1.00	22.80	B
ATOM	1601	CA	GLY	217	36.427	21.282	54.498	1.00	21.61	B
ATOM	1602	C	GLY	217	37.813	21.056	55.063	1.00	21.73	B
ATOM	1603	O	GLY	217	38.019	21.154	56.273	1.00	21.45	B
ATOM	1604	N	ALA	218	38.770	20.770	54.182	1.00	19.63	B
ATOM	1605	CA	ALA	218	40.146	20.522	54.607	1.00	20.23	B
ATOM	1606	CB	ALA	218	41.013	20.194	53.402	1.00	20.86	B
ATOM	1607	C	ALA	218	40.720	21.717	55.358	1.00	19.43	B
ATOM	1608	O	ALA	218	41.151	21.588	56.500	1.00	21.17	B
ATOM	1609	N	ALA	219	40.725	22.877	54.706	1.00	19.70	B
ATOM	1610	CA	ALA	219	41.248	24.111	55.299	1.00	18.89	B
ATOM	1611	CB	ALA	219	40.928	25.296	54.400	1.00	17.46	B
ATOM	1612	C	ALA	219	40.672	24.357	56.675	1.00	18.82	B
ATOM	1613	O	ALA	219	41.394	24.630	57.621	1.00	19.06	B
ATOM	1614	N	LYS	220	39.355	24.266	56.778	1.00	19.83	B
ATOM	1615	CA	LYS	220	38.698	24.501	58.049	1.00	21.65	B
ATOM	1616	CB	LYS	220	37.179	24.475	57.867	1.00	22.34	B
ATOM	1617	CG	LYS	220	36.416	24.906	59.101	1.00	25.89	B
ATOM	1618	CD	LYS	220	35.002	25.363	58.759	1.00	28.36	B
ATOM	1619	CE	LYS	220	34.296	25.886	60.002	1.00	28.81	B
ATOM	1620	NZ	LYS	220	32.888	26.286	59.732	1.00	27.62	B
ATOM	1621	C	LYS	220	39.145	23.486	59.101	1.00	21.92	B
ATOM	1622	O	LYS	220	39.199	23.807	60.278	1.00	23.01	B
ATOM	1623	N	ARG	221	39.478	22.268	58.672	1.00	21.66	B
ATOM	1624	CA	ARG	221	39.934	21.223	59.596	1.00	20.06	B
ATOM	1625	CB	ARG	221	40.015	19.878	58.882	1.00	22.12	B
ATOM	1626	CG	ARG	221	38.739	19.076	58.916	1.00	23.91	B
ATOM	1627	CD	ARG	221	38.952	17.787	58.173	1.00	26.21	B
ATOM	1628	NE	ARG	221	37.777	16.929	58.203	1.00	27.96	B
ATOM	1629	CZ	ARG	221	37.620	15.882	57.407	1.00	27.08	B
ATOM	1630	NH1	ARG	221	38.571	15.583	56.529	1.00	25.16	B
ATOM	1631	NH2	ARG	221	36.519	15.145	57.491	1.00	27.49	B
ATOM	1632	C	ARG	221	41.301	21.562	60.167	1.00	18.78	B
ATOM	1633	O	ARG	221	41.623	21.206	61.315	1.00	16.42	B
ATOM	1634	N	THR	222	42.101	22.238	59.350	1.00	15.19	B
ATOM	1635	CA	THR	222	43.433	22.659	59.741	1.00	15.22	B
ATOM	1636	CB	THR	222	44.119	23.409	58.593	1.00	16.99	B
ATOM	1637	OG1	THR	222	44.121	22.573	57.424	1.00	16.46	B
ATOM	1638	CG2	THR	222	45.534	23.796	58.977	1.00	14.73	B
ATOM	1639	C	THR	222	43.323	23.601	60.928	1.00	16.64	B
ATOM	1640	O	THR	222	44.046	23.461	61.920	1.00	16.06	B
ATOM	1641	N	THR	223	42.405	24.559	60.828	1.00	16.39	B
ATOM	1642	CA	THR	223	42.202	25.515	61.902	1.00	17.40	B
ATOM	1643	CB	THR	223	41.160	26.603	61.519	1.00	18.18	B
ATOM	1644	OG1	THR	223	39.839	26.125	61.780	1.00	22.16	B
ATOM	1645	CG2	THR	223	41.268	26.953	60.048	1.00	18.76	B
ATOM	1646	C	THR	223	41.708	24.757	63.134	1.00	17.96	B
ATOM	1647	O	THR	223	42.078	25.083	64.253	1.00	20.22	B
ATOM	1648	N	ALA	224	40.875	23.743	62.916	1.00	17.09	B
ATOM	1649	CA	ALA	224	40.348	22.953	64.027	1.00	17.61	B
ATOM	1650	CB	ALA	224	39.349	21.902	63.520	1.00	17.42	B
ATOM	1651	C	ALA	224	41.503	22.268	64.744	1.00	16.75	B
ATOM	1652	O	ALA	224	41.588	22.284	65.979	1.00	13.71	B
ATOM	1653	N	ALA	225	42.384	21.663	63.950	1.00	16.23	B
ATOM	1654	CA	ALA	225	43.551	20.980	64.486	1.00	15.92	B
ATOM	1655	CB	ALA	225	44.391	20.426	63.346	1.00	14.25	B
ATOM	1656	C	ALA	225	44.376	21.956	65.332	1.00	16.42	B
ATOM	1657	O	ALA	225	44.983	21.566	66.329	1.00	14.18	B
ATOM	1658	N	THR	226	44.385	23.231	64.931	1.00	18.14	B
ATOM	1659	CA	THR	226	45.135	24.261	65.666	1.00	18.36	B
ATOM	1660	CB	THR	226	45.205	25.606	64.894	1.00	19.59	B
ATOM	1661	OG1	THR	226	45.994	25.445	63.705	1.00	20.89	B
ATOM	1662	CG2	THR	226	45.821	26.696	65.775	1.00	18.63	B
ATOM	1663	C	THR	226	44.507	24.541	67.024	1.00	19.56	B
ATOM	1664	O	THR	226	45.214	24.765	68.000	1.00	22.00	B
ATOM	1665	N	LEU	227	43.178	24.527	67.074	1.00	19.70	B
ATOM	1666	CA	LEU	227	42.427	24.798	68.297	1.00	20.19	B
ATOM	1667	CB	LEU	227	41.011	25.291	67.943	1.00	22.99	B
ATOM	1668	CG	LEU	227	40.728	26.794	67.875	1.00	28.11	B
ATOM	1669	CD1	LEU	227	41.162	27.422	69.202	1.00	28.40	B
ATOM	1670	CD2	LEU	227	41.452	27.445	66.677	1.00	27.33	B

ATOM	1671	C	LEU	227	42.279	23.627	69.269	1.00	19.64	B
ATOM	1672	O	LEU	227	42.384	23.801	70.480	1.00	17.11	B
ATOM	1673	N	MET	228	42.021	22.440	68.727	1.00	21.48	B
ATOM	1674	CA	MET	228	41.807	21.253	69.557	1.00	21.62	B
ATOM	1675	CB	MET	228	40.465	20.627	69.174	1.00	21.31	B
ATOM	1676	CG	MET	228	39.286	21.542	69.510	1.00	22.62	B
ATOM	1677	SD	MET	228	37.764	21.286	68.570	1.00	28.36	B
ATOM	1678	CE	MET	228	37.979	22.463	67.223	1.00	25.23	B
ATOM	1679	C	MET	228	42.936	20.235	69.472	1.00	19.55	B
ATOM	1680	O	MET	228	43.364	19.884	68.392	1.00	19.08	B
ATOM	1681	N	ASN	229	43.404	19.764	70.628	1.00	19.30	B
ATOM	1682	CA	ASN	229	44.496	18.790	70.683	1.00	21.72	B
ATOM	1683	CB	ASN	229	44.902	18.512	72.140	1.00	21.27	B
ATOM	1684	CG	ASN	229	45.124	19.786	72.952	1.00	23.92	B
ATOM	1685	OD1	ASN	229	45.493	20.829	72.413	1.00	26.36	B
ATOM	1686	ND2	ASN	229	44.913	19.694	74.262	1.00	18.44	B
ATOM	1687	C	ASN	229	44.165	17.460	69.993	1.00	21.18	B
ATOM	1688	O	ASN	229	43.071	16.927	70.153	1.00	21.11	B
ATOM	1689	N	ALA	230	45.129	16.945	69.231	1.00	20.55	B
ATOM	1690	CA	ALA	230	44.975	15.683	68.510	1.00	21.88	B
ATOM	1691	CB	ALA	230	45.172	14.502	69.466	1.00	22.05	B
ATOM	1692	C	ALA	230	43.599	15.601	67.869	1.00	21.44	B
ATOM	1693	O	ALA	230	42.925	14.588	67.974	1.00	23.20	B
ATOM	1694	N	TYR	231	43.197	16.667	67.191	1.00	20.11	B
ATOM	1695	CA	TYR	231	41.878	16.708	66.568	1.00	21.54	B
ATOM	1696	CB	TYR	231	41.637	18.103	65.968	1.00	19.36	B
ATOM	1697	CG	TYR	231	40.280	18.276	65.322	1.00	14.20	B
ATOM	1698	CD1	TYR	231	40.106	18.061	63.956	1.00	10.71	B
ATOM	1699	CE1	TYR	231	38.852	18.173	63.369	1.00	9.05	B
ATOM	1700	CD2	TYR	231	39.159	18.613	66.085	1.00	14.00	B
ATOM	1701	CE2	TYR	231	37.900	18.725	65.503	1.00	11.47	B
ATOM	1702	CZ	TYR	231	37.757	18.505	64.152	1.00	9.28	B
ATOM	1703	OH	TYR	231	36.522	18.626	63.583	1.00	11.26	B
ATOM	1704	C	TYR	231	41.603	15.614	65.526	1.00	22.31	B
ATOM	1705	O	TYR	231	40.611	14.889	65.630	1.00	23.44	B
ATOM	1706	N	SER	232	42.481	15.482	64.538	1.00	21.31	B
ATOM	1707	CA	SER	232	42.286	14.487	63.486	1.00	21.21	B
ATOM	1708	CB	SER	232	43.382	14.614	62.424	1.00	19.70	B
ATOM	1709	OG	SER	232	44.658	14.355	62.980	1.00	22.28	B
ATOM	1710	C	SER	232	42.245	13.046	63.983	1.00	20.84	B
ATOM	1711	O	SER	232	41.718	12.165	63.303	1.00	21.67	B
ATOM	1712	N	SER	233	42.788	12.805	65.166	1.00	18.82	B
ATOM	1713	CA	SER	233	42.801	11.447	65.670	1.00	16.78	B
ATOM	1714	CB	SER	233	44.189	11.108	66.222	1.00	14.92	B
ATOM	1715	OG	SER	233	44.295	11.465	67.587	1.00	15.42	B
ATOM	1716	C	SER	233	41.745	11.193	66.741	1.00	17.60	B
ATOM	1717	O	SER	233	41.365	10.067	66.964	1.00	18.14	B
ATOM	1718	N	ARG	234	41.267	12.253	67.392	1.00	18.41	B
ATOM	1719	CA	ARG	234	40.266	12.113	68.450	1.00	18.22	B
ATOM	1720	CB	ARG	234	40.716	12.874	69.703	1.00	20.85	B
ATOM	1721	CG	ARG	234	41.207	11.975	70.809	1.00	26.63	B
ATOM	1722	CD	ARG	234	42.603	12.340	71.282	1.00	28.86	B
ATOM	1723	NE	ARG	234	42.624	13.522	72.138	1.00	28.89	B
ATOM	1724	CZ	ARG	234	43.641	13.853	72.927	1.00	30.32	B
ATOM	1725	NH1	ARG	234	44.724	13.089	72.969	1.00	29.87	B
ATOM	1726	NH2	ARG	234	43.571	14.941	73.683	1.00	29.28	B
ATOM	1727	C	ARG	234	38.858	12.559	68.065	1.00	18.79	B
ATOM	1728	O	ARG	234	37.986	12.639	68.914	1.00	18.55	B
ATOM	1729	N	SER	235	38.641	12.826	66.780	1.00	19.09	B
ATOM	1730	CA	SER	235	37.339	13.278	66.307	1.00	18.40	B
ATOM	1731	CB	SER	235	37.477	14.654	65.655	1.00	16.08	B
ATOM	1732	OG	SER	235	38.275	14.584	64.481	1.00	13.92	B
ATOM	1733	C	SER	235	36.694	12.314	65.312	1.00	18.89	B
ATOM	1734	O	SER	235	37.379	11.637	64.558	1.00	18.57	B
ATOM	1735	N	HIS	236	35.363	12.284	65.323	1.00	20.05	B
ATOM	1736	CA	HIS	236	34.571	11.445	64.427	1.00	20.67	B
ATOM	1737	CB	HIS	236	33.409	10.800	65.186	1.00	21.89	B
ATOM	1738	CG	HIS	236	33.819	10.092	66.439	1.00	22.09	B
ATOM	1739	CD2	HIS	236	33.733	10.462	67.740	1.00	22.95	B
ATOM	1740	ND1	HIS	236	34.406	8.847	66.433	1.00	22.44	B
ATOM	1741	CE1	HIS	236	34.663	8.480	67.677	1.00	24.61	B
ATOM	1742	NE2	HIS	236	34.265	9.441	68.489	1.00	23.56	B
ATOM	1743	C	HIS	236	33.994	12.353	63.345	1.00	21.61	B

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ATOM   1744  O   HIS   236      33.373  13.368  63.658  1.00 22.50      B
ATOM   1745  N   SER   237      34.195  12.000  62.080  1.00 20.87      B
ATOM   1746  CA  SER   237      33.673  12.813  60.992  1.00 21.41      B
ATOM   1747  CB  SER   237      34.811  13.241  60.061  1.00 21.79      B
ATOM   1748  OG  SER   237      35.388  12.121  59.411  1.00 21.23      B
ATOM   1749  C   SER   237      32.618  12.049  60.201  1.00 22.61      B
ATOM   1750  O   SER   237      32.863  10.939  59.749  1.00 23.35      B
ATOM   1751  N   VAL   238      31.440  12.648  60.053  1.00 21.59      B
ATOM   1752  CA  VAL   238      30.348  12.022  59.313  1.00 20.89      B
ATOM   1753  CB  VAL   238      29.106  11.821  60.234  1.00 22.16      B
ATOM   1754  CG1 VAL   238      28.807  13.104  60.977  1.00 24.21      B
ATOM   1755  CG2 VAL   238      27.886  11.395  59.419  1.00 18.41      B
ATOM   1756  C   VAL   238      29.967  12.872  58.103  1.00 18.95      B
ATOM   1757  O   VAL   238      29.157  13.772  58.205  1.00 18.39      B
ATOM   1758  N   PHE   239      30.586  12.577  56.962  1.00 19.38      B
ATOM   1759  CA  PHE   239      30.329  13.295  55.712  1.00 19.10      B
ATOM   1760  CB  PHE   239      31.501  13.115  54.735  1.00 16.63      B
ATOM   1761  CG  PHE   239      31.413  13.986  53.501  1.00 13.65      B
ATOM   1762  CD1 PHE   239      30.443  13.752  52.521  1.00 13.62      B
ATOM   1763  CD2 PHE   239      32.307  15.029  53.316  1.00 11.10      B
ATOM   1764  CE1 PHE   239      30.375  14.557  51.367  1.00 11.04      B
ATOM   1765  CE2 PHE   239      32.248  15.836  52.174  1.00 11.49      B
ATOM   1766  CZ  PHE   239      31.281  15.598  51.196  1.00 10.13      B
ATOM   1767  C   PHE   239      29.072  12.709  55.089  1.00 20.70      B
ATOM   1768  O   PHE   239      29.088  11.581  54.635  1.00 21.65      B
ATOM   1769  N   SER   240      27.992  13.487  55.056  1.00 19.79      B
ATOM   1770  CA  SER   240      26.737  12.999  54.489  1.00 20.02      B
ATOM   1771  CB  SER   240      25.568  13.303  55.430  1.00 17.99      B
ATOM   1772  OG  SER   240      25.714  12.651  56.682  1.00 13.88      B
ATOM   1773  C   SER   240      26.424  13.552  53.104  1.00 21.86      B
ATOM   1774  O   SER   240      26.721  14.684  52.796  1.00 22.91      B
ATOM   1775  N   VAL   241      25.818  12.720  52.271  1.00 23.30      B
ATOM   1776  CA  VAL   241      25.448  13.130  50.932  1.00 24.80      B
ATOM   1777  CB  VAL   241      26.432  12.581  49.884  1.00 24.40      B
ATOM   1778  CG1 VAL   241      26.805  11.139  50.226  1.00 26.22      B
ATOM   1779  CG2 VAL   241      25.807  12.668  48.494  1.00 19.02      B
ATOM   1780  C   VAL   241      24.035  12.646  50.619  1.00 26.53      B
ATOM   1781  O   VAL   241      23.806  11.465  50.433  1.00 27.95      B
ATOM   1782  N   THR   242      23.093  13.582  50.586  1.00 28.63      B
ATOM   1783  CA  THR   242      21.698  13.287  50.311  1.00 30.95      B
ATOM   1784  CB  THR   242      20.779  14.186  51.164  1.00 32.05      B
ATOM   1785  OG1 THR   242      20.997  13.901  52.555  1.00 33.54      B
ATOM   1786  CG2 THR   242      19.319  13.939  50.825  1.00 34.70      B
ATOM   1787  C   THR   242      21.393  13.490  48.828  1.00 32.32      B
ATOM   1788  O   THR   242      21.845  14.451  48.213  1.00 33.97      B
ATOM   1789  N   ILE   243      20.628  12.573  48.250  1.00 33.03      B
ATOM   1790  CA  ILE   243      20.293  12.660  46.837  1.00 33.83      B
ATOM   1791  CB  ILE   243      20.912  11.493  46.052  1.00 33.37      B
ATOM   1792  CG2 ILE   243      20.732  11.719  44.561  1.00 32.82      B
ATOM   1793  CG1 ILE   243      22.395  11.361  46.400  1.00 34.30      B
ATOM   1794  CD1 ILE   243      23.071  10.176  45.750  1.00 35.23      B
ATOM   1795  C   ILE   243      18.789  12.635  46.604  1.00 35.12      B
ATOM   1796  O   ILE   243      18.175  11.581  46.655  1.00 34.29      B
ATOM   1797  N   HIS   244      18.197  13.803  46.364  1.00 37.02      B
ATOM   1798  CA  HIS   244      16.766  13.878  46.097  1.00 38.10      B
ATOM   1799  CB  HIS   244      16.214  15.280  46.390  1.00 40.10      B
ATOM   1800  CG  HIS   244      16.190  15.635  47.845  1.00 42.80      B
ATOM   1801  CD2 HIS   244      15.219  15.493  48.781  1.00 43.38      B
ATOM   1802  ND1 HIS   244      17.271  16.192  48.496  1.00 44.55      B
ATOM   1803  CE1 HIS   244      16.968  16.376  49.770  1.00 44.18      B
ATOM   1804  NE2 HIS   244      15.729  15.960  49.968  1.00 43.01      B
ATOM   1805  C   HIS   244      16.569  13.545  44.624  1.00 38.58      B
ATOM   1806  O   HIS   244      17.113  14.216  43.754  1.00 38.74      B
ATOM   1807  N   MET   245      15.790  12.500  44.357  1.00 38.78      B
ATOM   1808  CA  MET   245      15.534  12.056  42.991  1.00 38.49      B
ATOM   1809  CB  MET   245      16.081  10.646  42.791  1.00 35.74      B
ATOM   1810  CG  MET   245      17.579  10.552  42.978  1.00 34.03      B
ATOM   1811  SD  MET   245      18.110   8.870  43.218  1.00 32.96      B
ATOM   1812  CE  MET   245      17.855   8.694  44.996  1.00 26.04      B
ATOM   1813  C   MET   245      14.058  12.083  42.618  1.00 39.24      B
ATOM   1814  O   MET   245      13.193  11.814  43.439  1.00 39.24      B
ATOM   1815  N   LYS   246      13.791  12.409  41.358  1.00 39.88      B
ATOM   1816  CA  LYS   246      12.430  12.477  40.855  1.00 40.90      B
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ATOM	1817	CB	LYS	246	11.910	13.916	40.915	1.00	42.86	B	
ATOM	1818	CG	LYS	246	10.453	14.080	40.467	1.00	45.41	B	
ATOM	1819	CD	LYS	246	10.140	15.516	40.018	1.00	47.23	B	
ATOM	1820	CE	LYS	246	10.383	16.538	41.134	1.00	49.08	B	
ATOM	1821	NZ	LYS	246	10.267	17.954	40.659	1.00	47.64	B	
ATOM	1822	C	LYS	246	12.406	11.994	39.414	1.00	41.15	B	
ATOM	1823	O	LYS	246	13.084	12.547	38.552	1.00	40.37	B	
ATOM	1824	N	GLU	247	11.622	10.954	39.163	1.00	40.39	B	
ATOM	1825	CA	GLU	247	11.496	10.414	37.821	1.00	40.56	B	
ATOM	1826	CB	GLU	247	12.010	8.977	37.769	1.00	39.14	B	
ATOM	1827	CG	GLU	247	11.479	8.090	38.866	1.00	37.23	B	
ATOM	1828	CD	GLU	247	12.390	6.916	39.118	1.00	36.86	B	
ATOM	1829	OE1	GLU	247	12.094	6.104	40.021	1.00	36.22	B	
ATOM	1830	OE2	GLU	247	13.410	6.813	38.406	1.00	36.77	B	
ATOM	1831	C	GLU	247	10.039	10.469	37.402	1.00	40.31	B	
ATOM	1832	O	GLU	247	9.142	10.304	38.220	1.00	39.86	B	
ATOM	1833	N	THR	248	9.820	10.720	36.117	1.00	40.83	B	
ATOM	1834	CA	THR	248	8.480	10.826	35.569	1.00	40.95	B	
ATOM	1835	CB	THR	248	8.339	12.123	34.736	1.00	40.97	B	
ATOM	1836	OG1	THR	248	8.804	13.238	35.507	1.00	41.15	B	
ATOM	1837	CG2	THR	248	6.886	12.363	34.358	1.00	40.88	B	
ATOM	1838	C	THR	248	8.143	9.625	34.690	1.00	40.36	B	
ATOM	1839	O	THR	248	8.799	9.380	33.684	1.00	40.50	B	
ATOM	1840	N	THR	249	7.111	8.885	35.086	1.00	39.94	B	
ATOM	1841	CA	THR	249	6.661	7.712	34.341	1.00	39.13	B	
ATOM	1842	CB	THR	249	5.537	6.976	35.086	1.00	39.64	B	
ATOM	1843	OG1	THR	249	4.307	7.686	34.897	1.00	37.39	B	
ATOM	1844	CG2	THR	249	5.846	6.894	36.575	1.00	38.52	B	
ATOM	1845	C	THR	249	6.115	8.132	32.980	1.00	39.50	B	
ATOM	1846	O	THR	249	5.943	9.311	32.713	1.00	39.71	B	
ATOM	1847	N	ILE	250	5.841	7.148	32.129	1.00	40.73	B	
ATOM	1848	CA	ILE	250	5.307	7.398	30.794	1.00	40.49	B	
ATOM	1849	CB	ILE	250	5.292	6.095	29.944	1.00	37.78	B	
ATOM	1850	CG2	ILE	250	4.244	5.135	30.472	1.00	37.42	B	
ATOM	1851	CG1	ILE	250	4.999	6.421	28.479	1.00	35.79	B	
ATOM	1852	CD1	ILE	250	5.125	5.238	27.552	1.00	33.62	B	
ATOM	1853	C	ILE	250	3.892	7.963	30.905	1.00	42.55	B	
ATOM	1854	O	ILE	250	3.361	8.534	29.953	1.00	43.05	B	
ATOM	1855	N	ASP	251	3.296	7.800	32.084	1.00	44.44	B	
ATOM	1856	CA	ASP	251	1.947	8.286	32.357	1.00	46.93	B	
ATOM	1857	CB	ASP	251	1.215	7.318	33.290	1.00	47.07	B	
ATOM	1858	CG	ASP	251	0.494	6.221	32.539	1.00	47.33	B	
ATOM	1859	OD1	ASP	251	0.034	5.257	33.190	1.00	47.89	B	
ATOM	1860	OD2	ASP	251	0.381	6.325	31.298	1.00	45.62	B	
ATOM	1861	C	ASP	251	1.965	9.675	32.987	1.00	48.37	B	
ATOM	1862	O	ASP	251	0.933	10.175	33.424	1.00	49.52	B	
ATOM	1863	N	GLY	252	3.145	10.286	33.038	1.00	49.00	B	
ATOM	1864	CA	GLY	252	3.275	11.612	33.609	1.00	48.84	B	
ATOM	1865	C	GLY	252	3.432	11.634	35.117	1.00	49.43	B	
ATOM	1866	O	GLY	252	3.856	12.638	35.675	1.00	49.95	B	
ATOM	1867	N	GLU	253	3.093	10.538	35.787	1.00	49.54	B	
ATOM	1868	CA	GLU	253	3.219	10.499	37.237	1.00	50.34	B	
ATOM	1869	CB	GLU	253	2.693	9.183	37.797	1.00	51.72	B	
ATOM	1870	CG	GLU	253	2.753	9.136	39.309	1.00	55.44	B	
ATOM	1871	CD	GLU	253	2.605	7.734	39.856	1.00	57.73	B	
ATOM	1872	OE1	GLU	253	2.703	7.561	41.091	1.00	59.23	B	
ATOM	1873	OE2	GLU	253	2.400	6.805	39.048	1.00	59.21	B	
ATOM	1874	C	GLU	253	4.671	10.678	37.661	1.00	49.73	B	
ATOM	1875	O	GLU	253	5.582	10.326	36.930	1.00	49.04	B	
ATOM	1876	N	GLU	254	4.878	11.229	38.851	1.00	49.71	B	
ATOM	1877	CA	GLU	254	6.230	11.445	39.346	1.00	50.40	B	
ATOM	1878	CB	GLU	254	6.452	12.927	39.629	1.00	51.91	B	
ATOM	1879	CG	GLU	254	7.036	13.680	38.448	1.00	56.74	B	
ATOM	1880	CD	GLU	254	6.579	15.124	38.397	1.00	59.63	B	
ATOM	1881	OE1	GLU	254	6.444	15.739	39.479	1.00	61.46	B	
ATOM	1882	OE2	GLU	254	6.363	15.642	37.276	1.00	60.48	B	
ATOM	1883	C	GLU	254	6.562	10.614	40.578	1.00	48.68	B	
ATOM	1884	O	GLU	254	5.812	10.579	41.546	1.00	47.25	B	
ATOM	1885	N	LEU	255	7.703	9.938	40.517	1.00	47.02	B	
ATOM	1886	CA	LEU	255	8.157	9.094	41.609	1.00	45.92	B	
ATOM	1887	CB	LEU	255	8.566	7.722	41.067	1.00	45.31	B	
ATOM	1888	CG	LEU	255	7.647	7.080	40.016	1.00	44.40	B	
ATOM	1889	CD1	LEU	255	8.308	5.837	39.454	1.00	43.92	B	

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ATOM   1890  CD2 LEU   255       6.294   6.747  40.621  1.00 43.09      B
ATOM   1891  C   LEU   255       9.353   9.780  42.250  1.00 46.31      B
ATOM   1892  O   LEU   255      10.346  10.044  41.580  1.00 46.88      B
ATOM   1893  N   VAL   256       9.255  10.069  43.545  1.00 46.34      B
ATOM   1894  CA  VAL   256      10.343  10.739  44.254  1.00 46.32      B
ATOM   1895  CB  VAL   256       9.837  12.012  44.988  1.00 46.60      B
ATOM   1896  CG1 VAL   256       9.447  13.075  43.971  1.00 46.43      B
ATOM   1897  CG2 VAL   256       8.642  11.679  45.870  1.00 46.46      B
ATOM   1898  C   VAL   256      11.049   9.835  45.258  1.00 45.32      B
ATOM   1899  O   VAL   256      10.428   9.287  46.158  1.00 45.96      B
ATOM   1900  N   LYS   257      12.359   9.687  45.077  1.00 44.55      B
ATOM   1901  CA  LYS   257      13.190   8.865  45.951  1.00 42.39      B
ATOM   1902  CB  LYS   257      13.997   7.852  45.133  1.00 43.00      B
ATOM   1903  CG  LYS   257      13.170   6.932  44.261  1.00 41.72      B
ATOM   1904  CD  LYS   257      14.058   6.001  43.457  1.00 38.34      B
ATOM   1905  CE  LYS   257      14.956   6.771  42.514  1.00 37.62      B
ATOM   1906  NZ  LYS   257      15.665   5.873  41.563  1.00 37.38      B
ATOM   1907  C   LYS   257      14.161   9.755  46.705  1.00 40.94      B
ATOM   1908  O   LYS   257      14.545  10.802  46.220  1.00 42.05      B
ATOM   1909  N   ILE   258      14.557   9.322  47.893  1.00 38.70      B
ATOM   1910  CA  ILE   258      15.498  10.082  48.699  1.00 35.70      B
ATOM   1911  CB  ILE   258      14.790  10.816  49.850  1.00 36.93      B
ATOM   1912  CG2 ILE   258      15.811  11.596  50.667  1.00 37.53      B
ATOM   1913  CG1 ILE   258      13.729  11.767  49.291  1.00 38.43      B
ATOM   1914  CD1 ILE   258      12.932  12.500  50.363  1.00 38.30      B
ATOM   1915  C   ILE   258      16.541   9.142  49.285  1.00 33.73      B
ATOM   1916  O   ILE   258      16.257   8.388  50.209  1.00 32.97      B
ATOM   1917  N   GLY   259      17.746   9.186  48.731  1.00 31.67      B
ATOM   1918  CA  GLY   259      18.815   8.338  49.219  1.00 30.51      B
ATOM   1919  C   GLY   259      19.874   9.136  49.956  1.00 29.55      B
ATOM   1920  O   GLY   259      20.363  10.138  49.442  1.00 30.38      B
ATOM   1921  N   LYS   260      20.230   8.692  51.159  1.00 27.15      B
ATOM   1922  CA  LYS   260      21.239   9.377  51.958  1.00 26.83      B
ATOM   1923  CB  LYS   260      20.603   9.940  53.240  1.00 24.21      B
ATOM   1924  CG  LYS   260      21.518  10.858  54.037  1.00 19.17      B
ATOM   1925  CD  LYS   260      20.833  11.362  55.289  1.00 17.68      B
ATOM   1926  CE  LYS   260      21.768  12.219  56.124  1.00 16.42      B
ATOM   1927  NZ  LYS   260      21.115  12.662  57.378  1.00 16.56      B
ATOM   1928  C   LYS   260      22.394   8.437  52.318  1.00 27.97      B
ATOM   1929  O   LYS   260      22.184   7.357  52.864  1.00 30.85      B
ATOM   1930  N   LEU   261      23.616   8.859  52.011  1.00 26.40      B
ATOM   1931  CA  LEU   261      24.792   8.056  52.306  1.00 24.54      B
ATOM   1932  CB  LEU   261      25.587   7.830  51.019  1.00 23.41      B
ATOM   1933  CG  LEU   261      26.989   7.243  51.175  1.00 23.40      B
ATOM   1934  CD1 LEU   261      26.922   5.920  51.941  1.00 20.72      B
ATOM   1935  CD2 LEU   261      27.599   7.045  49.798  1.00 20.51      B
ATOM   1936  C   LEU   261      25.685   8.715  53.362  1.00 23.98      B
ATOM   1937  O   LEU   261      26.117   9.836  53.198  1.00 22.95      B
ATOM   1938  N   ASN   262      25.953   8.000  54.448  1.00 22.99      B
ATOM   1939  CA  ASN   262      26.799   8.529  55.511  1.00 21.81      B
ATOM   1940  CB  ASN   262      26.138   8.303  56.874  1.00 19.98      B
ATOM   1941  CG  ASN   262      24.730   8.872  56.945  1.00 24.40      B
ATOM   1942  OD1 ASN   262      23.770   8.135  57.124  1.00 24.74      B
ATOM   1943  ND2 ASN   262      24.606  10.189  56.807  1.00 20.69      B
ATOM   1944  C   ASN   262      28.192   7.879  55.494  1.00 21.73      B
ATOM   1945  O   ASN   262      28.314   6.680  55.589  1.00 20.91      B
ATOM   1946  N   LEU   263      29.238   8.691  55.348  1.00 21.87      B
ATOM   1947  CA  LEU   263      30.611   8.191  55.338  1.00 20.99      B
ATOM   1948  CB  LEU   263      31.360   8.750  54.136  1.00 19.60      B
ATOM   1949  CG  LEU   263      30.578   8.470  52.856  1.00 20.68      B
ATOM   1950  CD1 LEU   263      31.187   9.220  51.710  1.00 22.18      B
ATOM   1951  CD2 LEU   263      30.557   6.972  52.584  1.00 20.91      B
ATOM   1952  C   LEU   263      31.262   8.650  56.630  1.00 21.08      B
ATOM   1953  O   LEU   263      31.631   9.793  56.753  1.00 20.87      B
ATOM   1954  N   VAL   264      31.397   7.734  57.586  1.00 22.31      B
ATOM   1955  CA  VAL   264      31.964   8.048  58.901  1.00 22.41      B
ATOM   1956  CB  VAL   264      31.119   7.378  60.042  1.00 22.70      B
ATOM   1957  CG1 VAL   264      31.373   8.082  61.372  1.00 22.08      B
ATOM   1958  CG2 VAL   264      29.627   7.398  59.691  1.00 23.20      B
ATOM   1959  C   VAL   264      33.425   7.645  59.112  1.00 23.23      B
ATOM   1960  O   VAL   264      33.776   6.482  58.994  1.00 25.35      B
ATOM   1961  N   ASP   265      34.262   8.625  59.443  1.00 23.36      B
ATOM   1962  CA  ASP   265      35.683   8.397  59.709  1.00 21.00      B
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ATOM	1963	CB	ASP	265	36.528	9.471	59.011	1.00	17.94	B
ATOM	1964	CG	ASP	265	38.024	9.311	59.258	1.00	18.29	B
ATOM	1965	OD1	ASP	265	38.429	8.960	60.384	1.00	17.19	B
ATOM	1966	OD2	ASP	265	38.806	9.554	58.322	1.00	15.43	B
ATOM	1967	C	ASP	265	35.840	8.501	61.230	1.00	21.25	B
ATOM	1968	O	ASP	265	36.208	9.550	61.758	1.00	22.30	B
ATOM	1969	N	LEU	266	35.552	7.406	61.928	1.00	19.20	B
ATOM	1970	CA	LEU	266	35.636	7.387	63.387	1.00	19.48	B
ATOM	1971	CB	LEU	266	35.269	5.991	63.913	1.00	17.26	B
ATOM	1972	CG	LEU	266	33.871	5.454	63.567	1.00	18.72	B
ATOM	1973	CD1	LEU	266	33.752	4.005	64.042	1.00	15.87	B
ATOM	1974	CD2	LEU	266	32.792	6.332	64.207	1.00	17.11	B
ATOM	1975	C	LEU	266	37.008	7.818	63.936	1.00	17.95	B
ATOM	1976	O	LEU	266	37.982	7.938	63.198	1.00	16.50	B
ATOM	1977	N	ALA	267	37.053	8.062	65.243	1.00	16.22	B
ATOM	1978	CA	ALA	267	38.284	8.458	65.920	1.00	17.36	B
ATOM	1979	CB	ALA	267	37.957	9.144	67.244	1.00	13.49	B
ATOM	1980	C	ALA	267	39.112	7.202	66.183	1.00	18.67	B
ATOM	1981	O	ALA	267	38.561	6.119	66.320	1.00	18.45	B
ATOM	1982	N	GLY	268	40.430	7.357	66.249	1.00	18.66	B
ATOM	1983	CA	GLY	268	41.291	6.226	66.507	1.00	20.51	B
ATOM	1984	C	GLY	268	40.738	5.336	67.604	1.00	22.52	B
ATOM	1985	O	GLY	268	40.123	5.815	68.545	1.00	22.16	B
ATOM	1986	N	SER	269	40.974	4.033	67.483	1.00	23.43	B
ATOM	1987	CA	SER	269	40.471	3.075	68.461	1.00	25.19	B
ATOM	1988	CB	SER	269	40.083	1.796	67.750	1.00	24.66	B
ATOM	1989	OG	SER	269	41.131	1.412	66.883	1.00	25.58	B
ATOM	1990	C	SER	269	41.446	2.739	69.584	1.00	26.21	B
ATOM	1991	O	SER	269	41.100	1.996	70.493	1.00	24.37	B
ATOM	1992	N	GLU	270	42.657	3.286	69.520	1.00	28.26	B
ATOM	1993	CA	GLU	270	43.664	3.029	70.546	1.00	31.89	B
ATOM	1994	CB	GLU	270	45.031	3.589	70.118	1.00	31.04	B
ATOM	1995	CG	GLU	270	45.140	5.113	70.033	1.00	28.41	B
ATOM	1996	CD	GLU	270	44.679	5.680	68.701	1.00	28.74	B
ATOM	1997	OE1	GLU	270	44.875	6.895	68.471	1.00	30.30	B
ATOM	1998	OE2	GLU	270	44.129	4.921	67.884	1.00	28.84	B
ATOM	1999	C	GLU	270	43.262	3.618	71.904	1.00	35.40	B
ATOM	2000	O	GLU	270	42.847	4.770	71.993	1.00	34.74	B
ATOM	2001	N	ASN	271	43.378	2.798	72.950	1.00	40.25	B
ATOM	2002	CA	ASN	271	43.039	3.192	74.324	1.00	44.12	B
ATOM	2003	CB	ASN	271	41.581	3.693	74.419	1.00	45.82	B
ATOM	2004	CG	ASN	271	40.546	2.600	74.147	1.00	46.03	B
ATOM	2005	OD1	ASN	271	39.347	2.845	74.224	1.00	45.22	B
ATOM	2006	ND2	ASN	271	41.011	1.395	73.829	1.00	47.11	B
ATOM	2007	C	ASN	271	43.246	2.039	75.307	1.00	45.92	B
ATOM	2008	O	ASN	271	43.668	0.938	74.922	1.00	46.63	B
ATOM	2009	N	ASN	287	41.544	11.757	79.480	1.00	56.32	B
ATOM	2010	CA	ASN	287	40.687	12.175	78.374	1.00	56.59	B
ATOM	2011	CB	ASN	287	41.514	12.914	77.315	1.00	58.79	B
ATOM	2012	CG	ASN	287	42.376	14.006	77.912	1.00	60.93	B
ATOM	2013	OD1	ASN	287	43.344	13.729	78.617	1.00	62.31	B
ATOM	2014	ND2	ASN	287	42.024	15.259	77.637	1.00	61.77	B
ATOM	2015	C	ASN	287	39.995	10.965	77.736	1.00	54.81	B
ATOM	2016	O	ASN	287	40.651	10.079	77.181	1.00	55.49	B
ATOM	2017	N	ILE	288	38.667	10.940	77.811	1.00	50.95	B
ATOM	2018	CA	ILE	288	37.889	9.838	77.252	1.00	46.25	B
ATOM	2019	CB	ILE	288	36.925	9.250	78.314	1.00	48.90	B
ATOM	2020	CG2	ILE	288	37.713	8.784	79.530	1.00	49.46	B
ATOM	2021	CG1	ILE	288	35.903	10.307	78.741	1.00	49.66	B
ATOM	2022	CD1	ILE	288	34.687	9.730	79.435	1.00	51.96	B
ATOM	2023	C	ILE	288	37.060	10.259	76.039	1.00	40.91	B
ATOM	2024	O	ILE	288	36.680	11.423	75.904	1.00	41.77	B
ATOM	2025	N	ASN	289	36.774	9.302	75.163	1.00	32.95	B
ATOM	2026	CA	ASN	289	35.979	9.582	73.976	1.00	26.09	B
ATOM	2027	CB	ASN	289	36.674	9.045	72.728	1.00	22.00	B
ATOM	2028	CG	ASN	289	36.093	9.612	71.444	1.00	19.37	B
ATOM	2029	OD1	ASN	289	36.819	9.927	70.521	1.00	19.84	B
ATOM	2030	ND2	ASN	289	34.774	9.725	71.382	1.00	17.42	B
ATOM	2031	C	ASN	289	34.624	8.927	74.154	1.00	22.64	B
ATOM	2032	O	ASN	289	34.394	7.805	73.718	1.00	22.38	B
ATOM	2033	N	GLN	290	33.726	9.652	74.806	1.00	20.05	B
ATOM	2034	CA	GLN	290	32.386	9.166	75.085	1.00	18.94	B
ATOM	2035	CB	GLN	290	31.542	10.299	75.659	1.00	20.27	B

ATOM	2036	CG	GLN	290	30.180	9.847	76.124	1.00	20.13	B
ATOM	2037	CD	GLN	290	30.273	8.777	77.182	1.00	20.41	B
ATOM	2038	OE1	GLN	290	29.311	8.067	77.441	1.00	22.39	B
ATOM	2039	NE2	GLN	290	31.435	8.662	77.806	1.00	20.99	B
ATOM	2040	C	GLN	290	31.652	8.526	73.899	1.00	18.42	B
ATOM	2041	O	GLN	290	30.945	7.543	74.068	1.00	15.37	B
ATOM	2042	N	SER	291	31.808	9.088	72.704	1.00	19.89	B
ATOM	2043	CA	SER	291	31.139	8.540	71.526	1.00	21.11	B
ATOM	2044	CB	SER	291	31.161	9.541	70.366	1.00	22.02	B
ATOM	2045	OG	SER	291	30.121	10.496	70.491	1.00	23.09	B
ATOM	2046	C	SER	291	31.757	7.212	71.090	1.00	22.87	B
ATOM	2047	O	SER	291	31.051	6.294	70.681	1.00	24.87	B
ATOM	2048	N	LEU	292	33.074	7.107	71.187	1.00	21.56	B
ATOM	2049	CA	LEU	292	33.741	5.878	70.812	1.00	21.17	B
ATOM	2050	CB	LEU	292	35.247	6.097	70.826	1.00	18.31	B
ATOM	2051	CG	LEU	292	36.074	5.053	70.089	1.00	18.27	B
ATOM	2052	CD1	LEU	292	35.653	4.994	68.625	1.00	13.66	B
ATOM	2053	CD2	LEU	292	37.548	5.418	70.218	1.00	17.97	B
ATOM	2054	C	LEU	292	33.345	4.785	71.818	1.00	21.64	B
ATOM	2055	O	LEU	292	32.914	3.703	71.454	1.00	19.24	B
ATOM	2056	N	LEU	293	33.481	5.100	73.098	1.00	22.14	B
ATOM	2057	CA	LEU	293	33.141	4.172	74.158	1.00	22.23	B
ATOM	2058	CB	LEU	293	33.374	4.841	75.513	1.00	22.95	B
ATOM	2059	CG	LEU	293	34.479	4.277	76.408	1.00	25.37	B
ATOM	2060	CD1	LEU	293	35.684	3.860	75.597	1.00	25.32	B
ATOM	2061	CD2	LEU	293	34.851	5.345	77.431	1.00	26.42	B
ATOM	2062	C	LEU	293	31.689	3.713	74.046	1.00	24.05	B
ATOM	2063	O	LEU	293	31.373	2.552	74.304	1.00	27.12	B
ATOM	2064	N	THR	294	30.807	4.622	73.647	1.00	23.43	B
ATOM	2065	CA	THR	294	29.396	4.293	73.534	1.00	22.37	B
ATOM	2066	CB	THR	294	28.554	5.580	73.487	1.00	22.35	B
ATOM	2067	OG1	THR	294	28.706	6.277	74.734	1.00	19.68	B
ATOM	2068	CG2	THR	294	27.090	5.275	73.270	1.00	19.85	B
ATOM	2069	C	THR	294	29.148	3.419	72.313	1.00	23.90	B
ATOM	2070	O	THR	294	28.276	2.561	72.325	1.00	26.74	B
ATOM	2071	N	LEU	295	29.938	3.628	71.268	1.00	24.08	B
ATOM	2072	CA	LEU	295	29.817	2.846	70.048	1.00	24.42	B
ATOM	2073	CB	LEU	295	30.822	3.332	69.004	1.00	22.92	B
ATOM	2074	CG	LEU	295	30.940	2.449	67.760	1.00	22.72	B
ATOM	2075	CD1	LEU	295	29.647	2.481	66.975	1.00	20.45	B
ATOM	2076	CD2	LEU	295	32.096	2.925	66.907	1.00	22.47	B
ATOM	2077	C	LEU	295	30.064	1.361	70.340	1.00	26.15	B
ATOM	2078	O	LEU	295	29.363	0.503	69.836	1.00	28.14	B
ATOM	2079	N	GLY	296	31.079	1.076	71.149	1.00	26.16	B
ATOM	2080	CA	GLY	296	31.391	-0.295	71.503	1.00	25.55	B
ATOM	2081	C	GLY	296	30.300	-0.915	72.361	1.00	25.59	B
ATOM	2082	O	GLY	296	29.898	-2.059	72.134	1.00	26.11	B
ATOM	2083	N	ARG	297	29.817	-0.162	73.346	1.00	22.71	B
ATOM	2084	CA	ARG	297	28.760	-0.660	74.217	1.00	22.15	B
ATOM	2085	CB	ARG	297	28.528	0.306	75.372	1.00	19.27	B
ATOM	2086	CG	ARG	297	29.719	0.450	76.284	1.00	20.29	B
ATOM	2087	CD	ARG	297	29.456	1.467	77.372	1.00	22.43	B
ATOM	2088	NE	ARG	297	30.639	1.658	78.201	1.00	26.34	B
ATOM	2089	CZ	ARG	297	31.226	2.833	78.407	1.00	24.22	B
ATOM	2090	NH1	ARG	297	30.729	3.921	77.838	1.00	23.11	B
ATOM	2091	NH2	ARG	297	32.306	2.918	79.178	1.00	18.73	B
ATOM	2092	C	ARG	297	27.449	-0.876	73.452	1.00	21.70	B
ATOM	2093	O	ARG	297	26.634	-1.674	73.844	1.00	20.12	B
ATOM	2094	N	VAL	298	27.255	-0.138	72.362	1.00	23.14	B
ATOM	2095	CA	VAL	298	26.046	-0.284	71.558	1.00	23.54	B
ATOM	2096	CB	VAL	298	25.845	0.924	70.613	1.00	22.84	B
ATOM	2097	CG1	VAL	298	24.742	0.634	69.582	1.00	18.86	B
ATOM	2098	CG2	VAL	298	25.477	2.146	71.432	1.00	19.90	B
ATOM	2099	C	VAL	298	26.150	-1.563	70.739	1.00	25.65	B
ATOM	2100	O	VAL	298	25.192	-2.325	70.643	1.00	27.92	B
ATOM	2101	N	ILE	299	27.317	-1.793	70.147	1.00	25.96	B
ATOM	2102	CA	ILE	299	27.516	-2.992	69.354	1.00	27.94	B
ATOM	2103	CB	ILE	299	28.880	-2.971	68.649	1.00	26.11	B
ATOM	2104	CG2	ILE	299	29.187	-4.330	68.053	1.00	24.74	B
ATOM	2105	CG1	ILE	299	28.862	-1.910	67.550	1.00	26.37	B
ATOM	2106	CD1	ILE	299	30.192	-1.704	66.889	1.00	28.12	B
ATOM	2107	C	ILE	299	27.413	-4.240	70.235	1.00	29.09	B
ATOM	2108	O	ILE	299	26.958	-5.284	69.791	1.00	28.96	B

ATOM	2109	N	THR	300	27.829	-4.112	71.490	1.00	29.82	B
ATOM	2110	CA	THR	300	27.771	-5.213	72.440	1.00	30.01	B
ATOM	2111	CB	THR	300	28.561	-4.877	73.706	1.00	29.27	B
ATOM	2112	OG1	THR	300	29.960	-4.842	73.392	1.00	30.68	B
ATOM	2113	CG2	THR	300	28.299	-5.900	74.796	1.00	28.12	B
ATOM	2114	C	THR	300	26.330	-5.517	72.821	1.00	32.39	B
ATOM	2115	O	THR	300	25.927	-6.675	72.902	1.00	33.67	B
ATOM	2116	N	ALA	301	25.552	-4.467	73.044	1.00	32.46	B
ATOM	2117	CA	ALA	301	24.157	-4.631	73.414	1.00	34.19	B
ATOM	2118	CB	ALA	301	23.584	-3.305	73.863	1.00	32.83	B
ATOM	2119	C	ALA	301	23.353	-5.182	72.238	1.00	35.75	B
ATOM	2120	O	ALA	301	22.348	-5.842	72.425	1.00	37.02	B
ATOM	2121	N	LEU	302	23.812	-4.899	71.024	1.00	36.43	B
ATOM	2122	CA	LEU	302	23.132	-5.352	69.817	1.00	38.14	B
ATOM	2123	CB	LEU	302	23.549	-4.488	68.622	1.00	38.00	B
ATOM	2124	CG	LEU	302	22.492	-3.555	68.031	1.00	39.25	B
ATOM	2125	CD1	LEU	302	21.823	-2.753	69.128	1.00	39.09	B
ATOM	2126	CD2	LEU	302	23.149	-2.630	67.016	1.00	38.56	B
ATOM	2127	C	LEU	302	23.428	-6.812	69.514	1.00	39.23	B
ATOM	2128	O	LEU	302	22.520	-7.594	69.249	1.00	39.50	B
ATOM	2129	N	VAL	303	24.709	-7.163	69.552	1.00	40.87	B
ATOM	2130	CA	VAL	303	25.161	-8.521	69.287	1.00	42.58	B
ATOM	2131	CB	VAL	303	26.706	-8.605	69.331	1.00	42.52	B
ATOM	2132	CG1	VAL	303	27.155	-10.051	69.270	1.00	43.58	B
ATOM	2133	CG2	VAL	303	27.301	-7.824	68.167	1.00	42.05	B
ATOM	2134	C	VAL	303	24.579	-9.496	70.306	1.00	44.19	B
ATOM	2135	O	VAL	303	24.048	-10.538	69.941	1.00	45.04	B
ATOM	2136	N	GLU	304	24.685	-9.145	71.584	1.00	45.93	B
ATOM	2137	CA	GLU	304	24.169	-9.973	72.667	1.00	48.10	B
ATOM	2138	CB	GLU	304	24.792	-9.541	73.998	1.00	47.26	B
ATOM	2139	CG	GLU	304	26.305	-9.707	74.041	1.00	46.33	B
ATOM	2140	CD	GLU	304	26.901	-9.334	75.382	1.00	46.65	B
ATOM	2141	OE1	GLU	304	28.139	-9.410	75.519	1.00	44.41	B
ATOM	2142	OE2	GLU	304	26.135	-8.968	76.302	1.00	47.42	B
ATOM	2143	C	GLU	304	22.649	-9.885	72.753	1.00	49.92	B
ATOM	2144	O	GLU	304	22.031	-10.492	73.612	1.00	50.02	B
ATOM	2145	N	ARG	305	22.061	-9.116	71.844	1.00	52.91	B
ATOM	2146	CA	ARG	305	20.614	-8.941	71.787	1.00	56.32	B
ATOM	2147	CB	ARG	305	19.952	-10.251	71.357	1.00	58.76	B
ATOM	2148	CG	ARG	305	20.300	-10.652	69.934	1.00	63.36	B
ATOM	2149	CD	ARG	305	19.501	-11.856	69.475	1.00	68.00	B
ATOM	2150	NE	ARG	305	19.718	-12.133	68.057	1.00	71.78	B
ATOM	2151	CZ	ARG	305	19.306	-11.344	67.068	1.00	73.93	B
ATOM	2152	NH1	ARG	305	18.650	-10.222	67.339	1.00	74.69	B
ATOM	2153	NH2	ARG	305	19.554	-11.675	65.807	1.00	75.22	B
ATOM	2154	C	ARG	305	19.981	-8.443	73.082	1.00	56.68	B
ATOM	2155	O	ARG	305	18.809	-8.699	73.340	1.00	56.68	B
ATOM	2156	N	THR	306	20.757	-7.728	73.892	1.00	57.02	B
ATOM	2157	CA	THR	306	20.248	-7.185	75.146	1.00	56.82	B
ATOM	2158	CB	THR	306	21.347	-6.426	75.912	1.00	56.33	B
ATOM	2159	OG1	THR	306	22.482	-7.281	76.095	1.00	56.76	B
ATOM	2160	CG2	THR	306	20.836	-5.975	77.272	1.00	56.64	B
ATOM	2161	C	THR	306	19.122	-6.213	74.812	1.00	57.35	B
ATOM	2162	O	THR	306	19.239	-5.421	73.881	1.00	58.12	B
ATOM	2163	N	PRO	307	18.011	-6.268	75.564	1.00	57.68	B
ATOM	2164	CD	PRO	307	17.750	-7.184	76.688	1.00	58.36	B
ATOM	2165	CA	PRO	307	16.861	-5.384	75.336	1.00	57.69	B
ATOM	2166	CB	PRO	307	15.959	-5.682	76.533	1.00	57.98	B
ATOM	2167	CG	PRO	307	16.241	-7.125	76.803	1.00	58.68	B
ATOM	2168	C	PRO	307	17.218	-3.898	75.237	1.00	56.99	B
ATOM	2169	O	PRO	307	16.684	-3.187	74.386	1.00	57.64	B
ATOM	2170	N	HIS	308	18.120	-3.439	76.105	1.00	55.27	B
ATOM	2171	CA	HIS	308	18.539	-2.034	76.123	1.00	53.51	B
ATOM	2172	CB	HIS	308	18.749	-1.565	77.567	1.00	55.71	B
ATOM	2173	CG	HIS	308	19.227	-0.150	77.677	1.00	58.12	B
ATOM	2174	CD2	HIS	308	20.385	0.367	78.155	1.00	59.12	B
ATOM	2175	ND1	HIS	308	18.475	0.925	77.252	1.00	58.97	B
ATOM	2176	CE1	HIS	308	19.148	2.043	77.464	1.00	58.91	B
ATOM	2177	NE2	HIS	308	20.310	1.732	78.012	1.00	59.24	B
ATOM	2178	C	HIS	308	19.813	-1.749	75.329	1.00	50.82	B
ATOM	2179	O	HIS	308	20.793	-2.472	75.433	1.00	50.26	B
ATOM	2180	N	VAL	309	19.780	-0.671	74.551	1.00	47.79	B
ATOM	2181	CA	VAL	309	20.921	-0.239	73.743	1.00	44.18	B

ATOM	2182	CB	VAL	309	20.619	-0.355	72.233	1.00	44.37	B
ATOM	2183	CG1	VAL	309	21.876	-0.067	71.427	1.00	43.69	B
ATOM	2184	CG2	VAL	309	20.076	-1.737	71.912	1.00	43.50	B
ATOM	2185	C	VAL	309	21.188	1.234	74.075	1.00	41.50	B
ATOM	2186	O	VAL	309	20.368	2.091	73.788	1.00	41.50	B
ATOM	2187	N	PRO	310	22.351	1.535	74.675	1.00	38.54	B
ATOM	2188	CD	PRO	310	23.440	0.586	74.968	1.00	37.32	B
ATOM	2189	CA	PRO	310	22.736	2.898	75.058	1.00	37.55	B
ATOM	2190	CB	PRO	310	23.983	2.669	75.909	1.00	36.77	B
ATOM	2191	CG	PRO	310	24.614	1.502	75.238	1.00	36.14	B
ATOM	2192	C	PRO	310	22.977	3.898	73.917	1.00	36.95	B
ATOM	2193	O	PRO	310	24.042	4.493	73.827	1.00	36.57	B
ATOM	2194	N	TYR	311	21.972	4.076	73.061	1.00	36.05	B
ATOM	2195	CA	TYR	311	22.047	5.012	71.940	1.00	34.95	B
ATOM	2196	CB	TYR	311	20.778	4.949	71.085	1.00	35.41	B
ATOM	2197	CG	TYR	311	20.603	3.711	70.245	1.00	36.70	B
ATOM	2198	CD1	TYR	311	21.603	3.289	69.374	1.00	35.89	B
ATOM	2199	CE1	TYR	311	21.433	2.161	68.578	1.00	36.91	B
ATOM	2200	CD2	TYR	311	19.416	2.973	70.300	1.00	36.75	B
ATOM	2201	CE2	TYR	311	19.234	1.844	69.508	1.00	36.61	B
ATOM	2202	CZ	TYR	311	20.247	1.442	68.651	1.00	36.85	B
ATOM	2203	OH	TYR	311	20.086	0.312	67.882	1.00	35.56	B
ATOM	2204	C	TYR	311	22.217	6.462	72.402	1.00	35.12	B
ATOM	2205	O	TYR	311	23.038	7.186	71.868	1.00	34.13	B
ATOM	2206	N	ARG	312	21.422	6.868	73.392	1.00	34.48	B
ATOM	2207	CA	ARG	312	21.444	8.237	73.906	1.00	34.28	B
ATOM	2208	CB	ARG	312	20.160	8.523	74.690	1.00	35.83	B
ATOM	2209	CG	ARG	312	18.882	8.227	73.935	1.00	41.17	B
ATOM	2210	CD	ARG	312	17.732	8.007	74.897	1.00	44.62	B
ATOM	2211	NE	ARG	312	16.596	7.341	74.263	1.00	48.42	B
ATOM	2212	CZ	ARG	312	15.608	6.747	74.926	1.00	51.08	B
ATOM	2213	NH1	ARG	312	15.610	6.732	76.254	1.00	50.32	B
ATOM	2214	NH2	ARG	312	14.618	6.163	74.259	1.00	51.58	B
ATOM	2215	C	ARG	312	22.638	8.593	74.787	1.00	33.03	B
ATOM	2216	O	ARG	312	22.701	9.699	75.317	1.00	34.26	B
ATOM	2217	N	GLU	313	23.581	7.669	74.953	1.00	29.69	B
ATOM	2218	CA	GLU	313	24.735	7.947	75.799	1.00	25.30	B
ATOM	2219	CB	GLU	313	25.200	6.655	76.481	1.00	24.49	B
ATOM	2220	CG	GLU	313	24.278	6.242	77.634	1.00	25.08	B
ATOM	2221	CD	GLU	313	24.677	4.946	78.327	1.00	23.59	B
ATOM	2222	OE1	GLU	313	25.883	4.722	78.553	1.00	23.79	B
ATOM	2223	OE2	GLU	313	23.775	4.156	78.665	1.00	23.87	B
ATOM	2224	C	GLU	313	25.898	8.646	75.089	1.00	23.89	B
ATOM	2225	O	GLU	313	26.963	8.806	75.659	1.00	23.12	B
ATOM	2226	N	SER	314	25.680	9.068	73.843	1.00	21.70	B
ATOM	2227	CA	SER	314	26.714	9.766	73.080	1.00	21.61	B
ATOM	2228	CB	SER	314	27.800	8.796	72.622	1.00	19.78	B
ATOM	2229	OG	SER	314	27.401	8.118	71.442	1.00	17.85	B
ATOM	2230	C	SER	314	26.124	10.466	71.861	1.00	23.50	B
ATOM	2231	O	SER	314	25.047	10.105	71.388	1.00	23.43	B
ATOM	2232	N	LYS	315	26.840	11.462	71.348	1.00	23.77	B
ATOM	2233	CA	LYS	315	26.367	12.204	70.186	1.00	24.56	B
ATOM	2234	CB	LYS	315	27.216	13.462	69.963	1.00	24.98	B
ATOM	2235	CG	LYS	315	27.295	14.394	71.165	1.00	25.63	B
ATOM	2236	CD	LYS	315	25.926	14.862	71.607	1.00	25.73	B
ATOM	2237	CE	LYS	315	26.034	15.834	72.774	1.00	26.31	B
ATOM	2238	NZ	LYS	315	26.660	17.123	72.353	1.00	30.29	B
ATOM	2239	C	LYS	315	26.416	11.335	68.939	1.00	24.22	B
ATOM	2240	O	LYS	315	25.498	11.338	68.138	1.00	25.98	B
ATOM	2241	N	LEU	316	27.503	10.591	68.787	1.00	23.22	B
ATOM	2242	CA	LEU	316	27.674	9.719	67.636	1.00	24.18	B
ATOM	2243	CB	LEU	316	29.039	9.022	67.711	1.00	24.13	B
ATOM	2244	CG	LEU	316	29.451	8.205	66.488	1.00	23.55	B
ATOM	2245	CD1	LEU	316	29.850	9.149	65.370	1.00	25.34	B
ATOM	2246	CD2	LEU	316	30.609	7.299	66.840	1.00	22.84	B
ATOM	2247	C	LEU	316	26.567	8.664	67.506	1.00	23.18	B
ATOM	2248	O	LEU	316	25.892	8.590	66.480	1.00	22.77	B
ATOM	2249	N	THR	317	26.369	7.855	68.543	1.00	22.09	B
ATOM	2250	CA	THR	317	25.346	6.817	68.470	1.00	22.50	B
ATOM	2251	CB	THR	317	25.459	5.809	69.651	1.00	20.87	B
ATOM	2252	OG1	THR	317	25.198	6.472	70.892	1.00	19.26	B
ATOM	2253	CG2	THR	317	26.848	5.192	69.682	1.00	20.16	B
ATOM	2254	C	THR	317	23.923	7.367	68.394	1.00	23.49	B

ATOM	2255	O	THR	317	23.025	6.684	67.929	1.00	23.95	B
ATOM	2256	N	ARG	318	23.723	8.606	68.836	1.00	23.82	B
ATOM	2257	CA	ARG	318	22.402	9.225	68.764	1.00	25.01	B
ATOM	2258	CB	ARG	318	22.317	10.426	69.705	1.00	28.63	B
ATOM	2259	CG	ARG	318	21.923	10.065	71.120	1.00	34.53	B
ATOM	2260	CD	ARG	318	22.260	11.179	72.094	1.00	38.92	B
ATOM	2261	NE	ARG	318	21.606	12.436	71.745	1.00	45.13	B
ATOM	2262	CZ	ARG	318	20.293	12.642	71.792	1.00	47.64	B
ATOM	2263	NH1	ARG	318	19.479	11.666	72.177	1.00	49.68	B
ATOM	2264	NH2	ARG	318	19.796	13.826	71.456	1.00	45.41	B
ATOM	2265	C	ARG	318	22.127	9.674	67.335	1.00	24.81	B
ATOM	2266	O	ARG	318	21.015	9.522	66.828	1.00	24.93	B
ATOM	2267	N	ILE	319	23.149	10.217	66.684	1.00	22.86	B
ATOM	2268	CA	ILE	319	23.001	10.688	65.313	1.00	23.60	B
ATOM	2269	CB	ILE	319	24.197	11.588	64.893	1.00	22.37	B
ATOM	2270	CG2	ILE	319	24.089	11.947	63.410	1.00	22.84	B
ATOM	2271	CG1	ILE	319	24.224	12.861	65.748	1.00	22.76	B
ATOM	2272	CD1	ILE	319	25.457	13.738	65.533	1.00	17.34	B
ATOM	2273	C	ILE	319	22.903	9.532	64.322	1.00	24.40	B
ATOM	2274	O	ILE	319	22.144	9.585	63.381	1.00	23.60	B
ATOM	2275	N	LEU	320	23.688	8.486	64.556	1.00	27.00	B
ATOM	2276	CA	LEU	320	23.725	7.331	63.664	1.00	28.83	B
ATOM	2277	CB	LEU	320	25.180	7.037	63.274	1.00	26.75	B
ATOM	2278	CG	LEU	320	26.035	8.151	62.668	1.00	28.19	B
ATOM	2279	CD1	LEU	320	27.479	7.720	62.710	1.00	27.81	B
ATOM	2280	CD2	LEU	320	25.601	8.459	61.237	1.00	26.81	B
ATOM	2281	C	LEU	320	23.098	6.053	64.220	1.00	30.42	B
ATOM	2282	O	LEU	320	23.501	4.957	63.841	1.00	31.06	B
ATOM	2283	N	GLN	321	22.097	6.188	65.085	1.00	32.73	B
ATOM	2284	CA	GLN	321	21.457	5.012	65.674	1.00	34.42	B
ATOM	2285	CB	GLN	321	20.466	5.419	66.777	1.00	35.23	B
ATOM	2286	CG	GLN	321	19.195	6.116	66.314	1.00	39.71	B
ATOM	2287	CD	GLN	321	18.320	6.569	67.488	1.00	42.32	B
ATOM	2288	OE1	GLN	321	17.881	5.755	68.298	1.00	42.09	B
ATOM	2289	NE2	GLN	321	18.069	7.877	67.577	1.00	44.14	B
ATOM	2290	C	GLN	321	20.758	4.102	64.663	1.00	33.44	B
ATOM	2291	O	GLN	321	20.677	2.901	64.868	1.00	34.48	B
ATOM	2292	N	ASP	322	20.261	4.666	63.569	1.00	32.24	B
ATOM	2293	CA	ASP	322	19.583	3.839	62.575	1.00	33.02	B
ATOM	2294	CB	ASP	322	18.780	4.693	61.595	1.00	32.22	B
ATOM	2295	CG	ASP	322	17.790	3.871	60.783	1.00	32.38	B
ATOM	2296	OD1	ASP	322	17.716	4.061	59.548	1.00	32.08	B
ATOM	2297	OD2	ASP	322	17.074	3.045	61.382	1.00	30.54	B
ATOM	2298	C	ASP	322	20.598	3.011	61.794	1.00	32.49	B
ATOM	2299	O	ASP	322	20.228	2.175	60.988	1.00	32.45	B
ATOM	2300	N	SER	323	21.880	3.274	62.030	1.00	32.77	B
ATOM	2301	CA	SER	323	22.951	2.547	61.361	1.00	30.97	B
ATOM	2302	CB	SER	323	24.122	3.480	61.067	1.00	28.95	B
ATOM	2303	OG	SER	323	23.837	4.320	59.959	1.00	27.41	B
ATOM	2304	C	SER	323	23.416	1.374	62.224	1.00	30.75	B
ATOM	2305	O	SER	323	24.171	0.517	61.783	1.00	29.17	B
ATOM	2306	N	LEU	324	22.966	1.352	63.470	1.00	30.45	B
ATOM	2307	CA	LEU	324	23.326	0.270	64.363	1.00	31.28	B
ATOM	2308	CB	LEU	324	24.046	0.809	65.606	1.00	31.28	B
ATOM	2309	CG	LEU	324	25.476	1.353	65.463	1.00	32.14	B
ATOM	2310	CD1	LEU	324	26.308	0.424	64.587	1.00	33.04	B
ATOM	2311	CD2	LEU	324	25.436	2.739	64.862	1.00	34.26	B
ATOM	2312	C	LEU	324	22.081	-0.511	64.771	1.00	31.54	B
ATOM	2313	O	LEU	324	21.468	-0.235	65.785	1.00	31.30	B
ATOM	2314	N	GLY	325	21.715	-1.490	63.950	1.00	33.73	B
ATOM	2315	CA	GLY	325	20.554	-2.311	64.249	1.00	33.79	B
ATOM	2316	C	GLY	325	19.244	-1.636	63.901	1.00	33.20	B
ATOM	2317	O	GLY	325	18.218	-1.905	64.517	1.00	33.16	B
ATOM	2318	N	GLY	326	19.286	-0.754	62.909	1.00	32.43	B
ATOM	2319	CA	GLY	326	18.090	-0.048	62.499	1.00	33.13	B
ATOM	2320	C	GLY	326	17.704	-0.420	61.088	1.00	34.86	B
ATOM	2321	O	GLY	326	17.905	-1.541	60.680	1.00	34.93	B
ATOM	2322	N	ARG	327	17.157	0.535	60.343	1.00	37.13	B
ATOM	2323	CA	ARG	327	16.748	0.278	58.974	1.00	38.94	B
ATOM	2324	CB	ARG	327	15.327	0.784	58.753	1.00	43.05	B
ATOM	2325	CG	ARG	327	14.278	0.034	59.559	1.00	49.59	B
ATOM	2326	CD	ARG	327	12.872	0.464	59.159	1.00	54.64	B
ATOM	2327	NE	ARG	327	12.071	-0.657	58.665	1.00	60.40	B

ATOM	2328	CZ	ARG	327	12.358	-1.380	57.583	1.00	62.77	B
ATOM	2329	NH1	ARG	327	13.441	-1.105	56.861	1.00	63.46	B
ATOM	2330	NH2	ARG	327	11.556	-2.377	57.219	1.00	61.73	B
ATOM	2331	C	ARG	327	17.686	0.887	57.934	1.00	38.03	B
ATOM	2332	O	ARG	327	17.249	1.289	56.869	1.00	37.61	B
ATOM	2333	N	THR	328	18.979	0.931	58.252	1.00	36.37	B
ATOM	2334	CA	THR	328	19.983	1.481	57.345	1.00	35.54	B
ATOM	2335	CB	THR	328	20.715	2.685	57.989	1.00	34.89	B
ATOM	2336	OG1	THR	328	19.798	3.762	58.194	1.00	35.66	B
ATOM	2337	CG2	THR	328	21.847	3.156	57.096	1.00	33.72	B
ATOM	2338	C	THR	328	21.040	0.442	56.974	1.00	34.98	B
ATOM	2339	O	THR	328	21.630	-0.170	57.848	1.00	36.65	B
ATOM	2340	N	ARG	329	21.274	0.252	55.678	1.00	33.43	B
ATOM	2341	CA	ARG	329	22.281	-0.704	55.226	1.00	33.67	B
ATOM	2342	CB	ARG	329	22.354	-0.752	53.696	1.00	35.61	B
ATOM	2343	CG	ARG	329	23.146	-1.938	53.156	1.00	40.29	B
ATOM	2344	CD	ARG	329	23.642	-1.691	51.736	1.00	45.76	B
ATOM	2345	NE	ARG	329	24.253	-2.877	51.133	1.00	51.83	B
ATOM	2346	CZ	ARG	329	25.297	-3.540	51.632	1.00	54.83	B
ATOM	2347	NH1	ARG	329	25.874	-3.148	52.761	1.00	54.64	B
ATOM	2348	NH2	ARG	329	25.772	-4.601	50.991	1.00	56.00	B
ATOM	2349	C	ARG	329	23.615	-0.218	55.764	1.00	30.92	B
ATOM	2350	O	ARG	329	24.034	0.871	55.452	1.00	33.46	B
ATOM	2351	N	THR	330	24.277	-1.028	56.573	1.00	28.10	B
ATOM	2352	CA	THR	330	25.541	-0.622	57.156	1.00	26.64	B
ATOM	2353	CB	THR	330	25.410	-0.524	58.691	1.00	25.12	B
ATOM	2354	OG1	THR	330	24.526	0.549	59.019	1.00	25.09	B
ATOM	2355	CG2	THR	330	26.760	-0.291	59.351	1.00	22.76	B
ATOM	2356	C	THR	330	26.723	-1.516	56.820	1.00	27.27	B
ATOM	2357	O	THR	330	26.602	-2.732	56.748	1.00	27.57	B
ATOM	2358	N	SER	331	27.868	-0.878	56.618	1.00	26.82	B
ATOM	2359	CA	SER	331	29.104	-1.567	56.308	1.00	26.67	B
ATOM	2360	CB	SER	331	29.442	-1.446	54.830	1.00	26.29	B
ATOM	2361	OG	SER	331	28.444	-2.072	54.052	1.00	31.25	B
ATOM	2362	C	SER	331	30.191	-0.907	57.125	1.00	26.05	B
ATOM	2363	O	SER	331	30.210	0.304	57.272	1.00	29.07	B
ATOM	2364	N	ILE	332	31.086	-1.712	57.677	1.00	24.35	B
ATOM	2365	CA	ILE	332	32.179	-1.190	58.472	1.00	20.58	B
ATOM	2366	CB	ILE	332	32.119	-1.704	59.917	1.00	16.78	B
ATOM	2367	CG2	ILE	332	33.367	-1.290	60.656	1.00	15.30	B
ATOM	2368	CG1	ILE	332	30.849	-1.195	60.605	1.00	14.73	B
ATOM	2369	CD1	ILE	332	30.641	-1.735	62.018	1.00	11.20	B
ATOM	2370	C	ILE	332	33.484	-1.646	57.855	1.00	22.60	B
ATOM	2371	O	ILE	332	33.635	-2.809	57.495	1.00	22.21	B
ATOM	2372	N	ILE	333	34.421	-0.718	57.713	1.00	23.08	B
ATOM	2373	CA	ILE	333	35.718	-1.046	57.148	1.00	21.26	B
ATOM	2374	CB	ILE	333	36.096	-0.086	56.011	1.00	20.77	B
ATOM	2375	CG2	ILE	333	37.401	-0.530	55.375	1.00	20.19	B
ATOM	2376	CG1	ILE	333	34.993	-0.065	54.950	1.00	22.76	B
ATOM	2377	CD1	ILE	333	35.297	0.826	53.738	1.00	19.77	B
ATOM	2378	C	ILE	333	36.736	-0.927	58.267	1.00	22.44	B
ATOM	2379	O	ILE	333	37.015	0.170	58.740	1.00	25.05	B
ATOM	2380	N	ALA	334	37.269	-2.061	58.708	1.00	22.25	B
ATOM	2381	CA	ALA	334	38.252	-2.080	59.783	1.00	21.24	B
ATOM	2382	CB	ALA	334	38.088	-3.351	60.605	1.00	21.16	B
ATOM	2383	C	ALA	334	39.667	-1.998	59.212	1.00	20.54	B
ATOM	2384	O	ALA	334	40.070	-2.850	58.452	1.00	21.75	B
ATOM	2385	N	THR	335	40.405	-0.952	59.582	1.00	18.02	B
ATOM	2386	CA	THR	335	41.772	-0.771	59.102	1.00	15.52	B
ATOM	2387	CB	THR	335	42.052	0.701	58.752	1.00	14.93	B
ATOM	2388	OG1	THR	335	41.551	1.558	59.794	1.00	16.56	B
ATOM	2389	CG2	THR	335	41.394	1.051	57.447	1.00	13.76	B
ATOM	2390	C	THR	335	42.780	-1.257	60.132	1.00	14.40	B
ATOM	2391	O	THR	335	42.586	-1.096	61.340	1.00	13.68	B
ATOM	2392	N	ILE	336	43.863	-1.849	59.641	1.00	15.75	B
ATOM	2393	CA	ILE	336	44.893	-2.409	60.506	1.00	16.07	B
ATOM	2394	CB	ILE	336	44.671	-3.936	60.702	1.00	14.75	B
ATOM	2395	CG2	ILE	336	43.346	-4.185	61.401	1.00	13.27	B
ATOM	2396	CG1	ILE	336	44.678	-4.662	59.348	1.00	15.22	B
ATOM	2397	CD1	ILE	336	44.726	-6.215	59.461	1.00	13.20	B
ATOM	2398	C	ILE	336	46.317	-2.186	59.999	1.00	17.99	B
ATOM	2399	O	ILE	336	46.534	-1.816	58.844	1.00	17.06	B
ATOM	2400	N	SER	337	47.280	-2.407	60.889	1.00	20.83	B

ATOM	2401	CA	SER	337	48.694	-2.250	60.570	1.00	23.58	B	
ATOM	2402	CB	SER	337	49.399	-1.491	61.685	1.00	22.57	B	
ATOM	2403	OG	SER	337	50.792	-1.737	61.645	1.00	21.86	B	
ATOM	2404	C	SER	337	49.395	-3.600	60.389	1.00	27.32	B	
ATOM	2405	O	SER	337	49.123	-4.548	61.122	1.00	27.36	B	
ATOM	2406	N	PRO	338	50.320	-3.688	59.416	1.00	28.03	B	
ATOM	2407	CD	PRO	338	50.612	-2.678	58.383	1.00	29.38	B	
ATOM	2408	CA	PRO	338	51.063	-4.919	59.147	1.00	30.56	B	
ATOM	2409	CB	PRO	338	51.485	-4.743	57.698	1.00	29.47	B	
ATOM	2410	CG	PRO	338	51.804	-3.283	57.657	1.00	28.25	B	
ATOM	2411	C	PRO	338	52.274	-5.047	60.074	1.00	31.99	B	
ATOM	2412	O	PRO	338	52.903	-6.083	60.131	1.00	32.55	B	
ATOM	2413	N	ALA	339	52.586	-3.972	60.790	1.00	33.15	B	
ATOM	2414	CA	ALA	339	53.732	-3.955	61.690	1.00	34.44	B	
ATOM	2415	CB	ALA	339	54.051	-2.518	62.109	1.00	35.58	B	
ATOM	2416	C	ALA	339	53.505	-4.816	62.918	1.00	35.05	B	
ATOM	2417	O	ALA	339	52.391	-4.956	63.386	1.00	35.58	B	
ATOM	2418	N	SER	340	54.585	-5.380	63.447	1.00	36.34	B	
ATOM	2419	CA	SER	340	54.479	-6.236	64.615	1.00	36.42	B	
ATOM	2420	CB	SER	340	55.694	-7.162	64.717	1.00	36.55	B	
ATOM	2421	OG	SER	340	56.891	-6.431	64.909	1.00	37.23	B	
ATOM	2422	C	SER	340	54.324	-5.457	65.914	1.00	36.18	B	
ATOM	2423	O	SER	340	53.769	-5.969	66.871	1.00	36.17	B	
ATOM	2424	N	LEU	341	54.803	-4.220	65.957	1.00	36.13	B	
ATOM	2425	CA	LEU	341	54.664	-3.453	67.190	1.00	38.21	B	
ATOM	2426	CB	LEU	341	55.663	-2.296	67.239	1.00	40.75	B	
ATOM	2427	CG	LEU	341	55.293	-1.011	66.500	1.00	44.27	B	
ATOM	2428	CD1	LEU	341	56.054	0.160	67.121	1.00	44.94	B	
ATOM	2429	CD2	LEU	341	55.597	-1.158	65.011	1.00	45.97	B	
ATOM	2430	C	LEU	341	53.244	-2.912	67.337	1.00	36.82	B	
ATOM	2431	O	LEU	341	52.944	-2.185	68.259	1.00	37.65	B	
ATOM	2432	N	ASN	342	52.376	-3.288	66.408	1.00	36.59	B	
ATOM	2433	CA	ASN	342	50.983	-2.856	66.416	1.00	35.71	B	
ATOM	2434	CB	ASN	342	50.636	-2.219	65.071	1.00	34.64	B	
ATOM	2435	CG	ASN	342	51.343	-0.903	64.865	1.00	34.11	B	
ATOM	2436	OD1	ASN	342	51.904	-0.649	63.808	1.00	32.85	B	
ATOM	2437	ND2	ASN	342	51.315	-0.052	65.888	1.00	32.94	B	
ATOM	2438	C	ASN	342	50.084	-4.048	66.661	1.00	35.91	B	
ATOM	2439	O	ASN	342	48.860	-3.958	66.561	1.00	37.26	B	
ATOM	2440	N	LEU	343	50.720	-5.164	66.993	1.00	34.56	B	
ATOM	2441	CA	LEU	343	50.033	-6.419	67.244	1.00	32.49	B	
ATOM	2442	CB	LEU	343	51.019	-7.433	67.836	1.00	31.23	B	
ATOM	2443	CG	LEU	343	50.546	-8.858	68.135	1.00	31.25	B	
ATOM	2444	CD1	LEU	343	50.001	-8.944	69.548	1.00	32.82	B	
ATOM	2445	CD2	LEU	343	49.504	-9.286	67.101	1.00	30.64	B	
ATOM	2446	C	LEU	343	48.817	-6.295	68.140	1.00	30.37	B	
ATOM	2447	O	LEU	343	47.714	-6.608	67.732	1.00	29.24	B	
ATOM	2448	N	GLU	344	49.023	-5.831	69.364	1.00	30.64	B	
ATOM	2449	CA	GLU	344	47.922	-5.710	70.307	1.00	32.19	B	
ATOM	2450	CB	GLU	344	48.442	-5.121	71.619	1.00	34.78	B	
ATOM	2451	CG	GLU	344	47.460	-5.189	72.761	1.00	42.18	B	
ATOM	2452	CD	GLU	344	48.107	-4.861	74.099	1.00	47.80	B	
ATOM	2453	OE1	GLU	344	48.743	-3.785	74.209	1.00	48.41	B	
ATOM	2454	OE2	GLU	344	47.982	-5.686	75.036	1.00	49.00	B	
ATOM	2455	C	GLU	344	46.736	-4.899	69.760	1.00	30.46	B	
ATOM	2456	O	GLU	344	45.600	-5.355	69.802	1.00	29.53	B	
ATOM	2457	N	GLU	345	46.991	-3.707	69.234	1.00	29.30	B	
ATOM	2458	CA	GLU	345	45.901	-2.891	68.703	1.00	29.30	B	
ATOM	2459	CB	GLU	345	46.393	-1.477	68.349	1.00	29.27	B	
ATOM	2460	CG	GLU	345	46.618	-0.581	69.565	1.00	29.72	B	
ATOM	2461	CD	GLU	345	45.337	-0.285	70.330	1.00	30.47	B	
ATOM	2462	OE1	GLU	345	45.429	0.193	71.482	1.00	33.09	B	
ATOM	2463	OE2	GLU	345	44.241	-0.521	69.786	1.00	30.71	B	
ATOM	2464	C	GLU	345	45.277	-3.556	67.476	1.00	27.38	B	
ATOM	2465	O	GLU	345	44.082	-3.423	67.233	1.00	28.53	B	
ATOM	2466	N	THR	346	46.084	-4.283	66.711	1.00	24.59	B	
ATOM	2467	CA	THR	346	45.576	-4.979	65.530	1.00	23.55	B	
ATOM	2468	CB	THR	346	46.717	-5.588	64.721	1.00	22.82	B	
ATOM	2469	OG1	THR	346	47.503	-4.534	64.147	1.00	24.62	B	
ATOM	2470	CG2	THR	346	46.173	-6.473	63.618	1.00	23.82	B	
ATOM	2471	C	THR	346	44.597	-6.083	65.937	1.00	22.61	B	
ATOM	2472	O	THR	346	43.617	-6.343	65.252	1.00	22.38	B	
ATOM	2473	N	LEU	347	44.873	-6.732	67.062	1.00	23.16	B	

ATOM	2474	CA	LEU	347	44.002	-7.790	67.561	1.00	23.19	B
ATOM	2475	CB	LEU	347	44.678	-8.568	68.696	1.00	21.66	B
ATOM	2476	CG	LEU	347	45.955	-9.346	68.374	1.00	22.14	B
ATOM	2477	CD1	LEU	347	46.393	-10.118	69.613	1.00	20.42	B
ATOM	2478	CD2	LEU	347	45.718	-10.293	67.210	1.00	22.20	B
ATOM	2479	C	LEU	347	42.679	-7.203	68.063	1.00	23.83	B
ATOM	2480	O	LEU	347	41.617	-7.712	67.732	1.00	25.14	B
ATOM	2481	N	SER	348	42.743	-6.135	68.854	1.00	21.92	B
ATOM	2482	CA	SER	348	41.518	-5.530	69.368	1.00	23.12	B
ATOM	2483	CB	SER	348	41.839	-4.306	70.215	1.00	21.23	B
ATOM	2484	OG	SER	348	42.491	-4.707	71.402	1.00	27.13	B
ATOM	2485	C	SER	348	40.582	-5.144	68.238	1.00	22.86	B
ATOM	2486	O	SER	348	39.384	-5.348	68.331	1.00	22.12	B
ATOM	2487	N	THR	349	41.156	-4.596	67.172	1.00	23.05	B
ATOM	2488	CA	THR	349	40.391	-4.186	66.005	1.00	25.38	B
ATOM	2489	CB	THR	349	41.309	-3.483	64.988	1.00	25.69	B
ATOM	2490	OG1	THR	349	41.656	-2.185	65.495	1.00	28.94	B
ATOM	2491	CG2	THR	349	40.627	-3.334	63.639	1.00	26.37	B
ATOM	2492	C	THR	349	39.714	-5.387	65.344	1.00	27.04	B
ATOM	2493	O	THR	349	38.502	-5.396	65.164	1.00	25.10	B
ATOM	2494	N	LEU	350	40.505	-6.399	64.988	1.00	29.73	B
ATOM	2495	CA	LEU	350	39.971	-7.610	64.352	1.00	32.43	B
ATOM	2496	CB	LEU	350	41.112	-8.602	64.087	1.00	32.67	B
ATOM	2497	CG	LEU	350	41.782	-8.523	62.709	1.00	33.86	B
ATOM	2498	CD1	LEU	350	41.867	-7.089	62.243	1.00	35.72	B
ATOM	2499	CD2	LEU	350	43.160	-9.140	62.777	1.00	34.30	B
ATOM	2500	C	LEU	350	38.880	-8.268	65.203	1.00	32.13	B
ATOM	2501	O	LEU	350	37.869	-8.736	64.693	1.00	31.89	B
ATOM	2502	N	GLU	351	39.104	-8.286	66.510	1.00	32.99	B
ATOM	2503	CA	GLU	351	38.163	-8.869	67.452	1.00	33.24	B
ATOM	2504	CB	GLU	351	38.807	-8.951	68.837	1.00	36.70	B
ATOM	2505	CG	GLU	351	38.014	-9.772	69.821	1.00	44.06	B
ATOM	2506	CD	GLU	351	37.791	-11.179	69.309	1.00	47.54	B
ATOM	2507	OE1	GLU	351	38.805	-11.848	68.982	1.00	48.67	B
ATOM	2508	OE2	GLU	351	36.610	-11.599	69.228	1.00	48.07	B
ATOM	2509	C	GLU	351	36.901	-8.009	67.519	1.00	31.83	B
ATOM	2510	O	GLU	351	35.778	-8.532	67.584	1.00	32.55	B
ATOM	2511	N	TYR	352	37.097	-6.690	67.503	1.00	29.09	B
ATOM	2512	CA	TYR	352	35.997	-5.727	67.550	1.00	25.10	B
ATOM	2513	CB	TYR	352	36.561	-4.318	67.758	1.00	23.54	B
ATOM	2514	CG	TYR	352	35.537	-3.220	67.970	1.00	23.52	B
ATOM	2515	CD1	TYR	352	34.862	-2.642	66.893	1.00	21.07	B
ATOM	2516	CE1	TYR	352	33.952	-1.601	67.086	1.00	22.50	B
ATOM	2517	CD2	TYR	352	35.271	-2.734	69.254	1.00	23.10	B
ATOM	2518	CE2	TYR	352	34.366	-1.699	69.464	1.00	22.61	B
ATOM	2519	CZ	TYR	352	33.712	-1.134	68.377	1.00	25.05	B
ATOM	2520	OH	TYR	352	32.840	-0.085	68.577	1.00	29.15	B
ATOM	2521	C	TYR	352	35.169	-5.790	66.262	1.00	23.04	B
ATOM	2522	O	TYR	352	33.957	-5.819	66.309	1.00	21.96	B
ATOM	2523	N	ALA	353	35.841	-5.821	65.117	1.00	21.97	B
ATOM	2524	CA	ALA	353	35.155	-5.883	63.826	1.00	24.73	B
ATOM	2525	CB	ALA	353	36.163	-5.732	62.692	1.00	21.20	B
ATOM	2526	C	ALA	353	34.380	-7.192	63.663	1.00	26.52	B
ATOM	2527	O	ALA	353	33.283	-7.210	63.119	1.00	25.94	B
ATOM	2528	N	HIS	354	34.978	-8.282	64.138	1.00	30.11	B
ATOM	2529	CA	HIS	354	34.375	-9.607	64.052	1.00	32.42	B
ATOM	2530	CB	HIS	354	35.334	-10.660	64.626	1.00	35.26	B
ATOM	2531	CG	HIS	354	34.939	-12.073	64.317	1.00	38.11	B
ATOM	2532	CD2	HIS	354	34.416	-13.045	65.103	1.00	38.24	B
ATOM	2533	ND1	HIS	354	35.045	-12.614	63.053	1.00	39.29	B
ATOM	2534	CE1	HIS	354	34.600	-13.858	63.072	1.00	38.94	B
ATOM	2535	NE2	HIS	354	34.213	-14.143	64.303	1.00	39.79	B
ATOM	2536	C	HIS	354	33.050	-9.642	64.811	1.00	33.09	B
ATOM	2537	O	HIS	354	32.048	-10.127	64.297	1.00	33.51	B
ATOM	2538	N	ARG	355	33.053	-9.122	66.034	1.00	33.22	B
ATOM	2539	CA	ARG	355	31.847	-9.091	66.852	1.00	35.31	B
ATOM	2540	CB	ARG	355	32.145	-8.470	68.220	1.00	38.27	B
ATOM	2541	CG	ARG	355	32.976	-9.320	69.155	1.00	41.93	B
ATOM	2542	CD	ARG	355	33.322	-8.539	70.416	1.00	44.68	B
ATOM	2543	NE	ARG	355	32.132	-8.099	71.142	1.00	46.84	B
ATOM	2544	CZ	ARG	355	31.299	-8.915	71.781	1.00	48.76	B
ATOM	2545	NH1	ARG	355	31.523	-10.222	71.785	1.00	48.40	B
ATOM	2546	NH2	ARG	355	30.243	-8.423	72.420	1.00	47.82	B

ATOM	2547	C	ARG	355	30.740	-8.281	66.173	1.00	35.52	B
ATOM	2548	O	ARG	355	29.564	-8.610	66.297	1.00	36.07	B
ATOM	2549	N	ALA	356	31.124	-7.228	65.454	1.00	33.02	B
ATOM	2550	CA	ALA	356	30.146	-6.374	64.789	1.00	31.19	B
ATOM	2551	CB	ALA	356	30.837	-5.156	64.206	1.00	31.50	B
ATOM	2552	C	ALA	356	29.342	-7.089	63.704	1.00	31.06	B
ATOM	2553	O	ALA	356	28.259	-6.645	63.343	1.00	28.55	B
ATOM	2554	N	LYS	357	29.880	-8.197	63.194	1.00	31.69	B
ATOM	2555	CA	LYS	357	29.215	-8.973	62.144	1.00	33.26	B
ATOM	2556	CB	LYS	357	30.060	-10.198	61.768	1.00	35.45	B
ATOM	2557	CG	LYS	357	31.491	-9.906	61.350	1.00	36.26	B
ATOM	2558	CD	LYS	357	31.791	-10.458	59.956	1.00	39.94	B
ATOM	2559	CE	LYS	357	31.524	-11.968	59.851	1.00	40.54	B
ATOM	2560	NZ	LYS	357	32.455	-12.795	60.666	1.00	40.76	B
ATOM	2561	C	LYS	357	27.816	-9.447	62.552	1.00	33.43	B
ATOM	2562	O	LYS	357	26.911	-9.512	61.724	1.00	33.00	B
ATOM	2563	N	ASN	358	27.654	-9.773	63.833	1.00	34.87	B
ATOM	2564	CA	ASN	358	26.381	-10.253	64.379	1.00	36.60	B
ATOM	2565	CB	ASN	358	26.621	-10.942	65.724	1.00	37.20	B
ATOM	2566	CG	ASN	358	27.509	-12.159	65.606	1.00	38.73	B
ATOM	2567	OD1	ASN	358	28.105	-12.602	66.589	1.00	40.28	B
ATOM	2568	ND2	ASN	358	27.598	-12.713	64.404	1.00	38.63	B
ATOM	2569	C	ASN	358	25.320	-9.170	64.574	1.00	37.65	B
ATOM	2570	O	ASN	358	24.431	-9.322	65.406	1.00	38.18	B
ATOM	2571	N	ILE	359	25.413	-8.076	63.825	1.00	38.97	B
ATOM	2572	CA	ILE	359	24.430	-7.003	63.951	1.00	40.85	B
ATOM	2573	CB	ILE	359	25.088	-5.608	63.869	1.00	40.68	B
ATOM	2574	CG2	ILE	359	24.014	-4.529	63.858	1.00	40.16	B
ATOM	2575	CG1	ILE	359	26.019	-5.402	65.066	1.00	40.61	B
ATOM	2576	CD1	ILE	359	26.871	-4.161	64.970	1.00	39.58	B
ATOM	2577	C	ILE	359	23.391	-7.132	62.847	1.00	41.96	B
ATOM	2578	O	ILE	359	23.729	-7.227	61.671	1.00	42.22	B
ATOM	2579	N	LEU	360	22.122	-7.140	63.241	1.00	43.88	B
ATOM	2580	CA	LEU	360	21.024	-7.276	62.293	1.00	46.61	B
ATOM	2581	CB	LEU	360	19.952	-8.212	62.864	1.00	48.74	B
ATOM	2582	CG	LEU	360	19.660	-9.524	62.123	1.00	52.19	B
ATOM	2583	CD1	LEU	360	18.886	-10.456	63.043	1.00	51.91	B
ATOM	2584	CD2	LEU	360	18.870	-9.248	60.836	1.00	53.68	B
ATOM	2585	C	LEU	360	20.406	-5.927	61.966	1.00	46.77	B
ATOM	2586	O	LEU	360	19.969	-5.211	62.854	1.00	46.72	B
ATOM	2587	N	ASN	361	20.380	-5.586	60.681	1.00	47.32	B
ATOM	2588	CA	ASN	361	19.805	-4.320	60.242	1.00	48.31	B
ATOM	2589	CB	ASN	361	20.834	-3.502	59.458	1.00	47.61	B
ATOM	2590	CG	ASN	361	21.795	-2.743	60.360	1.00	48.03	B
ATOM	2591	OD1	ASN	361	22.423	-1.777	59.933	1.00	48.30	B
ATOM	2592	ND2	ASN	361	21.913	-3.175	61.609	1.00	47.01	B
ATOM	2593	C	ASN	361	18.563	-4.526	59.387	1.00	49.65	B
ATOM	2594	O	ASN	361	18.294	-5.627	58.919	1.00	51.43	B
ATOM	2595	N	LYS	362	17.821	-3.443	59.180	1.00	51.11	B
ATOM	2596	CA	LYS	362	16.586	-3.452	58.400	1.00	50.99	B
ATOM	2597	CB	LYS	362	16.883	-3.545	56.896	1.00	50.83	B
ATOM	2598	CG	LYS	362	17.289	-2.229	56.253	1.00	49.23	B
ATOM	2599	CD	LYS	362	17.117	-2.268	54.740	1.00	48.73	B
ATOM	2600	CE	LYS	362	15.643	-2.244	54.329	1.00	47.35	B
ATOM	2601	NZ	LYS	362	14.989	-0.914	54.515	1.00	44.68	B
ATOM	2602	C	LYS	362	15.659	-4.588	58.814	1.00	51.66	B
ATOM	2603	O	LYS	362	15.211	-5.329	57.913	1.00	52.28	B
ATOM	2604	OXT	LYS	362	15.387	-4.712	60.031	1.00	50.87	B
ATOM	2605	MG	MG	2602	43.651	10.621	59.419	1.00	27.37	
ATOM	2606	PB	ADP	2600	44.241	7.165	60.136	1.00	25.05	ADP
ATOM	2607	O1B	ADP	2600	44.666	7.765	61.419	1.00	26.27	ADP
ATOM	2608	O2B	ADP	2600	43.842	5.630	60.325	1.00	30.28	ADP
ATOM	2609	O3B	ADP	2600	43.097	7.920	59.552	1.00	28.27	ADP
ATOM	2610	PA	ADP	2600	45.608	7.818	57.697	1.00	39.43	ADP
ATOM	2611	O1A	ADP	2600	44.613	7.286	56.772	1.00	38.84	ADP
ATOM	2612	O2A	ADP	2600	45.462	9.276	57.778	1.00	41.49	ADP
ATOM	2613	O3A	ADP	2600	45.426	7.167	59.121	1.00	32.30	ADP
ATOM	2614	O5*	ADP	2600	47.084	7.550	57.187	1.00	39.41	ADP
ATOM	2615	C5*	ADP	2600	48.157	6.858	57.828	1.00	42.82	ADP
ATOM	2616	C4*	ADP	2600	49.374	6.940	56.825	1.00	45.97	ADP
ATOM	2617	O4*	ADP	2600	49.399	5.696	56.137	1.00	46.62	ADP
ATOM	2618	C3*	ADP	2600	49.266	8.021	55.715	1.00	46.20	ADP
ATOM	2619	O3*	ADP	2600	50.512	8.717	55.502	1.00	49.03	ADP

ATOM	2620	C2*	ADP	2600	48.810	7.296	54.462	1.00	46.75	ADP
ATOM	2621	O2*	ADP	2600	49.235	7.921	53.240	1.00	48.13	ADP
ATOM	2622	C1*	ADP	2600	49.328	5.886	54.701	1.00	47.35	ADP
ATOM	2623	N9	ADP	2600	48.435	4.815	54.144	1.00	48.03	ADP
ATOM	2624	C8	ADP	2600	47.417	4.221	54.811	1.00	47.72	ADP
ATOM	2625	N7	ADP	2600	46.839	3.328	54.046	1.00	48.56	ADP
ATOM	2626	C5	ADP	2600	47.454	3.316	52.892	1.00	49.10	ADP
ATOM	2627	C6	ADP	2600	47.308	2.603	51.707	1.00	49.07	ADP
ATOM	2628	N6	ADP	2600	46.350	1.680	51.610	1.00	49.43	ADP
ATOM	2629	N1	ADP	2600	48.159	2.844	50.628	1.00	50.04	ADP
ATOM	2630	C2	ADP	2600	49.152	3.776	50.684	1.00	48.98	ADP
ATOM	2631	N3	ADP	2600	49.301	4.478	51.842	1.00	50.49	ADP
ATOM	2632	C4	ADP	2600	48.491	4.283	52.944	1.00	48.96	ADP
ATOM	2633	C1	2-7	1	37.376	16.487	53.441	1.00	31.12	2-7
ATOM	2634	C2	2-7	1	38.554	16.442	52.639	1.00	31.01	2-7
ATOM	2635	C3	2-7	1	38.554	15.433	51.622	1.00	31.01	2-7
ATOM	2636	C4	2-7	1	37.388	14.559	51.530	1.00	29.91	2-7
ATOM	2637	C5	2-7	1	36.248	14.570	52.396	1.00	29.25	2-7
ATOM	2638	C6	2-7	1	36.296	15.546	53.415	1.00	30.61	2-7
ATOM	2639	C10	2-7	1	39.708	15.357	50.686	1.00	30.99	2-7
ATOM	2640	C11	2-7	1	40.272	16.598	50.056	1.00	33.35	2-7
ATOM	2641	N12	2-7	1	41.446	16.158	49.317	1.00	33.73	2-7
ATOM	2642	C13	2-7	1	41.189	14.730	49.013	1.00	31.60	2-7
ATOM	2643	C14	2-7	1	40.419	14.175	50.202	1.00	30.03	2-7
ATOM	2644	C17	2-7	1	41.032	14.136	47.645	1.00	28.72	2-7
ATOM	2645	C19	2-7	1	42.014	13.131	47.164	1.00	27.73	2-7
ATOM	2646	C20	2-7	1	41.952	12.752	45.765	1.00	26.29	2-7
ATOM	2647	C21	2-7	1	40.984	13.380	44.878	1.00	26.40	2-7
ATOM	2648	C22	2-7	1	39.931	14.256	45.351	1.00	27.79	2-7
ATOM	2649	C23	2-7	1	39.958	14.694	46.762	1.00	27.64	2-7
ATOM	2650	C29	2-7	1	42.438	17.110	49.102	1.00	34.81	2-7
ATOM	2651	N30	2-7	1	43.717	16.767	49.283	1.00	35.06	2-7
ATOM	2652	C31	2-7	1	44.603	17.929	49.086	1.00	31.67	2-7
ATOM	2653	C35	2-7	1	44.177	15.446	49.734	1.00	32.58	2-7
ATOM	2654	O39	2-7	1	42.187	18.279	48.762	1.00	35.09	2-7
ATOM	2655	F40	2-7	1	37.369	13.692	50.535	1.00	32.42	2-7
ATOM	2656	F41	2-7	1	37.291	17.497	54.277	1.00	33.09	2-7
ATOM	2657	O	HOH	2	38.630	10.603	62.535	1.00	3.96	S
ATOM	2658	O	HOH	3	28.064	20.853	56.798	1.00	15.26	S
ATOM	2659	O	HOH	4	43.423	-1.052	63.682	1.00	6.84	S
ATOM	2660	O	HOH	5	41.471	9.650	60.748	1.00	28.56	S
ATOM	2661	O	HOH	6	53.043	-17.874	61.146	1.00	22.21	S
ATOM	2662	O	HOH	8	43.351	23.546	43.947	1.00	14.88	S
ATOM	2663	O	HOH	11	31.538	6.420	79.791	1.00	20.07	S
ATOM	2664	O	HOH	12	44.364	1.570	53.833	1.00	33.76	S
ATOM	2665	O	HOH	13	42.141	-0.803	71.483	1.00	23.37	S
ATOM	2666	O	HOH	17	50.048	-0.508	68.644	1.00	38.33	S
ATOM	2667	O	HOH	18	42.525	8.183	64.075	1.00	31.71	S
ATOM	2668	O	HOH	20	49.961	-5.304	63.635	1.00	28.76	S
ATOM	2669	O	HOH	21	52.974	11.228	41.771	1.00	27.37	S
ATOM	2670	O	HOH	23	44.880	17.208	64.490	1.00	19.87	S
ATOM	2671	O	HOH	25	33.865	11.390	57.228	1.00	14.50	S
ATOM	2672	O	HOH	26	42.746	19.345	56.865	1.00	19.80	S
ATOM	2673	O	HOH	27	43.217	3.216	42.636	1.00	29.84	S
ATOM	2674	O	HOH	28	47.542	18.783	69.096	1.00	24.56	S
ATOM	2675	O	HOH	29	29.606	-8.997	58.639	1.00	41.51	S
ATOM	2676	O	HOH	30	38.143	15.249	61.346	1.00	12.36	S
ATOM	2677	O	HOH	31	47.769	14.311	41.568	1.00	24.48	S
ATOM	2678	O	HOH	32	22.227	19.477	42.995	1.00	35.68	S
ATOM	2679	O	HOH	34	38.077	4.715	80.434	1.00	19.14	S
ATOM	2680	O	HOH	35	27.208	25.794	60.457	1.00	30.49	S
ATOM	2681	O	HOH	40	45.874	21.711	68.966	1.00	14.93	S
ATOM	2682	O	HOH	42	37.931	3.241	64.945	1.00	21.80	S
ATOM	2683	O	HOH	44	33.173	12.293	71.900	1.00	38.67	S
ATOM	2684	O	HOH	45	38.986	3.636	49.470	1.00	20.20	S
ATOM	2685	O	HOH	46	35.162	19.890	41.213	1.00	25.42	S
ATOM	2686	O	HOH	52	22.755	-3.615	56.949	1.00	33.63	S
ATOM	2687	O	HOH	53	27.917	6.206	79.432	1.00	19.49	S
ATOM	2688	O	HOH	55	37.862	4.182	47.024	1.00	13.89	S
ATOM	2689	O	HOH	57	31.462	4.272	82.519	1.00	37.59	S
ATOM	2690	O	HOH	59	38.826	12.586	58.140	1.00	18.34	S
ATOM	2691	O	HOH	60	27.879	4.380	76.644	1.00	24.90	S
ATOM	2692	O	HOH	61	45.041	10.037	53.740	1.00	42.66	S

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ATOM   2693  O   HOH    62      28.763  26.533  62.454  1.00 35.09      S
ATOM   2694  O   HOH    66      38.448  -0.512  37.739  1.00 44.71      S
ATOM   2695  O   HOH    67      31.394  24.733  63.775  1.00 40.50      S
ATOM   2696  O   HOH    68      40.487   5.787  72.041  1.00 37.21      S
ATOM   2697  O   HOH    69      52.548  19.976  38.009  1.00 24.27      S
ATOM   2698  O   HOH    70      40.043  -1.641  68.804  1.00 21.10      S
ATOM   2699  O   HOH    71      21.370  18.117  39.097  1.00 47.89      S
ATOM   2700  O   HOH    73      45.431  -1.388  51.309  1.00 36.21      S
ATOM   2701  O   HOH    74      12.109   0.216  54.870  1.00 45.32      S
ATOM   2702  O   HOH    78      41.390   5.467  40.236  1.00 31.36      S
ATOM   2703  O   HOH    79      38.398 -10.202  49.709  1.00 28.25      S
ATOM   2704  O   HOH    84      46.457  -1.971  63.989  1.00 20.69      S
ATOM   2705  O   HOH    87       2.291   6.433  36.064  1.00 27.27      S
ATOM   2706  O   HOH    88      46.187   3.359  74.292  1.00 30.60      S
ATOM   2707  O   HOH    89      51.911   4.577  56.634  1.00 44.94      S
ATOM   2708  O   HOH    90      45.811  18.580  66.703  1.00 26.87      S
ATOM   2709  O   HOH    91      47.734  13.013  72.702  1.00 32.94      S
ATOM   2710  O   HOH    92      23.555  15.386  53.064  1.00 29.56      S
ATOM   2711  O   HOH    93      43.670  -2.643  73.172  1.00 27.18      S
ATOM   2712  O   HOH    94      27.978  20.947  70.487  1.00 41.48      S
ATOM   2713  O   HOH    95      44.678  -7.048  71.862  1.00 24.48      S
ATOM   2714  O   HOH    97      37.124   2.776  73.009  1.00 36.39      S
ATOM   2715  O   HOH    98      32.730  25.500  47.607  1.00 42.43      S
ATOM   2716  O   HOH   101      46.793  22.739  62.116  1.00 28.62      S
ATOM   2717  O   HOH   104      20.079  21.304  46.635  1.00 44.83      S
ATOM   2718  O   HOH   105      30.653  -3.670  75.744  1.00 35.11      S
ATOM   2719  O   HOH   106      46.987  13.182  34.815  1.00 16.99      S
ATOM   2720  O   HOH   109      43.794   0.066  55.803  1.00 30.02      S
ATOM   2721  O   HOH   111      25.208   9.102  28.662  1.00 32.86      S
ATOM   2722  O   HOH   113      44.655  15.401  59.741  1.00 25.68      S
ATOM   2723  O   HOH   115      18.285  12.456  33.587  1.00 30.40      S
ATOM   2724  O   HOH   116      47.999  -0.217  48.915  1.00 36.92      S
ATOM   2725  O   HOH   117      23.508  25.313  66.864  1.00 47.95      S
ATOM   2726  O   HOH   119      27.220 -14.904  55.904  1.00 35.41      S
ATOM   2727  O   HOH   120      47.343   8.255  68.520  1.00 37.89      S
ATOM   2728  O   HOH   128      28.608  -6.298  48.882  1.00 26.00      S
ATOM   2729  O   HOH   132       6.107  15.208  42.672  1.00 30.09      S
ATOM   2730  O   HOH   133      26.812  14.766  57.900  1.00 17.88      S
ATOM   2731  O   HOH   135      46.950  10.746  67.779  1.00 31.59      S
ATOM   2732  O   HOH   136      24.332   1.606  79.565  1.00 28.86      S
ATOM   2733  O   HOH   138      50.215   2.473  62.680  1.00 35.95      S
ATOM   2734  O   HOH   139      22.069  24.748  54.683  1.00 25.56      S
ATOM   2735  O   HOH   140      44.497 -18.491  58.486  1.00 49.65      S
ATOM   2736  O   HOH   141      15.900  -4.594  62.687  1.00 33.93      S
ATOM   2737  O   HOH   143      14.793  -3.866  47.507  1.00 45.81      S
END
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TABLE 4

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REMARK FILENAME="Compound 4-2a_2dpb.pdb"
!CRYST    69.200   79.400  159.200  90.00  90.00  90.00 P212121
ATOM   2605  CB  LYS    17      24.472 -12.132  60.197  1.00 50.92      B
ATOM   2606  CG  LYS    17      23.137 -12.714  59.720  1.00 53.46      B
ATOM   2607  CD  LYS    17      22.777 -12.276  58.298  1.00 55.17      B
ATOM   2608  CE  LYS    17      23.486 -13.129  57.240  1.00 56.45      B
ATOM   2609  NZ  LYS    17      24.977 -13.074  57.341  1.00 55.91      B
ATOM   2610  C   LYS    17      24.464  -9.793  59.322  1.00 46.31      B
ATOM   2611  O   LYS    17      25.371  -9.870  58.525  1.00 47.38      B
ATOM   2612  N   LYS    17      23.273 -10.326  61.434  1.00 49.07      B
ATOM   2613  CA  LYS    17      24.459 -10.640  60.578  1.00 48.39      B
ATOM   2614  N   ASN    18      23.441  -8.969  59.167  1.00 44.08      B
ATOM   2615  CA  ASN    18      23.346  -8.128  57.990  1.00 42.08      B
ATOM   2616  CB  ASN    18      22.016  -7.375  58.014  1.00 42.87      B
ATOM   2617  CG  ASN    18      21.059  -7.856  56.934  1.00 45.64      B
ATOM   2618  OD1 ASN    18      21.222  -7.538  55.748  1.00 47.65      B
ATOM   2619  ND2 ASN    18      20.068  -8.642  57.331  1.00 46.01      B
ATOM   2620  C   ASN    18      24.508  -7.150  57.750  1.00 40.28      B
ATOM   2621  O   ASN    18      24.895  -6.921  56.596  1.00 42.10      B
ATOM   2622  N   ILE    19      25.077  -6.584  58.810  1.00 36.30      B
ATOM   2623  CA  ILE    19      26.171  -5.618  58.668  1.00 32.31      B
ATOM   2624  CB  ILE    19      26.495  -4.982  60.043  1.00 33.05      B
ATOM   2625  CG2 ILE    19      26.959  -6.042  61.012  1.00 34.85      B
ATOM   2626  CG1 ILE    19      27.599  -3.938  59.905  1.00 33.89      B
ATOM   2627  CD1 ILE    19      27.845  -3.169  61.165  1.00 32.25      B
ATOM   2628  C   ILE    19      27.464  -6.184  58.058  1.00 28.41      B
ATOM   2629  O   ILE    19      28.021  -7.161  58.574  1.00 29.07      B
ATOM   2630  N   GLN    20      27.934  -5.566  56.967  1.00 22.29      B
ATOM   2631  CA  GLN    20      29.174  -5.986  56.285  1.00 15.95      B
ATOM   2632  CB  GLN    20      29.216  -5.493  54.839  1.00 14.82      B
ATOM   2633  CG  GLN    20      30.526  -5.834  54.127  1.00 14.68      B
ATOM   2634  CD  GLN    20      30.589  -5.290  52.715  1.00 13.60      B
ATOM   2635  OE1 GLN    20      30.540  -4.089  52.514  1.00 13.47      B
ATOM   2636  NE2 GLN    20      30.720  -6.173  51.737  1.00 13.04      B
ATOM   2637  C   GLN    20      30.450  -5.437  56.952  1.00 13.25      B
ATOM   2638  O   GLN    20      30.566  -4.239  57.180  1.00 12.33      B
ATOM   2639  N   VAL    21      31.394  -6.328  57.254  1.00  9.34      B
ATOM   2640  CA  VAL    21      32.656  -5.941  57.880  1.00  6.24      B
ATOM   2641  CB  VAL    21      32.775  -6.537  59.296  1.00  5.92      B
ATOM   2642  CG1 VAL    21      34.094  -6.144  59.934  1.00  3.44      B
ATOM   2643  CG2 VAL    21      31.616  -6.056  60.138  1.00  7.73      B
ATOM   2644  C   VAL    21      33.868  -6.396  57.052  1.00  5.09      B
ATOM   2645  O   VAL    21      34.031  -7.569  56.766  1.00  4.24      B
ATOM   2646  N   VAL    22      34.715  -5.454  56.659  1.00  3.75      B
ATOM   2647  CA  VAL    22      35.893  -5.805  55.879  1.00  4.12      B
ATOM   2648  CB  VAL    22      35.819  -5.226  54.420  1.00  3.36      B
ATOM   2649  CG1 VAL    22      34.566  -5.731  53.703  1.00  3.16      B
ATOM   2650  CG2 VAL    22      35.823  -3.717  54.452  1.00  2.87      B
ATOM   2651  C   VAL    22      37.157  -5.305  56.553  1.00  6.20      B
ATOM   2652  O   VAL    22      37.122  -4.365  57.352  1.00  6.79      B
ATOM   2653  N   VAL    23      38.271  -5.946  56.223  1.00  4.46      B
ATOM   2654  CA  VAL    23      39.559  -5.585  56.785  1.00  4.23      B
ATOM   2655  CB  VAL    23      40.195  -6.830  57.477  1.00  4.02      B
ATOM   2656  CG1 VAL    23      41.555  -6.511  58.081  1.00  1.86      B
ATOM   2657  CG2 VAL    23      39.268  -7.319  58.550  1.00  5.77      B
ATOM   2658  C   VAL    23      40.505  -5.037  55.710  1.00  4.46      B
ATOM   2659  O   VAL    23      40.553  -5.531  54.586  1.00  4.66      B
ATOM   2660  N   ARG    24      41.251  -3.998  56.057  1.00  7.29      B
ATOM   2661  CA  ARG    24      42.228  -3.436  55.128  1.00  9.87      B
ATOM   2662  CB  ARG    24      41.793  -2.092  54.531  1.00  6.53      B
ATOM   2663  CG  ARG    24      42.744  -1.662  53.425  1.00  6.89      B
ATOM   2664  CD  ARG    24      42.401  -0.306  52.837  1.00  7.91      B
ATOM   2665  NE  ARG    24      43.142  -0.040  51.603  1.00  4.86      B
ATOM   2666  CZ  ARG    24      43.041   1.095  50.909  1.00  3.46      B
ATOM   2667  NH1 ARG    24      42.228   2.056  51.329  1.00  1.00      B
ATOM   2668  NH2 ARG    24      43.773   1.287  49.814  1.00  1.00      B
ATOM   2669  C   ARG    24      43.541  -3.179  55.856  1.00 13.03      B
ATOM   2670  O   ARG    24      43.586  -2.374  56.791  1.00 13.45      B
ATOM   2671  N   CYS    25      44.593  -3.873  55.421  1.00 13.86      B
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ATOM	2672	CA	CYS	25	45.928	-3.742	55.996	1.00	16.78	B	
ATOM	2673	CB	CYS	25	46.646	-5.088	55.932	1.00	14.53	B	
ATOM	2674	SG	CYS	25	48.149	-5.147	56.865	1.00	15.92	B	
ATOM	2675	C	CYS	25	46.743	-2.706	55.216	1.00	17.93	B	
ATOM	2676	O	CYS	25	46.793	-2.743	53.991	1.00	19.83	B	
ATOM	2677	N	ARG	26	47.369	-1.774	55.922	1.00	20.13	B	
ATOM	2678	CA	ARG	26	48.186	-0.779	55.242	1.00	23.56	B	
ATOM	2679	CB	ARG	26	48.410	0.441	56.122	1.00	23.04	B	
ATOM	2680	CG	ARG	26	49.018	0.108	57.480	1.00	25.34	B	
ATOM	2681	CD	ARG	26	49.478	1.335	58.248	1.00	25.85	B	
ATOM	2682	NE	ARG	26	50.882	1.635	57.970	1.00	27.66	B	
ATOM	2683	CZ	ARG	26	51.876	1.425	58.830	1.00	29.35	B	
ATOM	2684	NH1	ARG	26	51.620	0.914	60.030	1.00	28.00	B	
ATOM	2685	NH2	ARG	26	53.126	1.729	58.494	1.00	29.65	B	
ATOM	2686	C	ARG	26	49.566	-1.360	54.924	1.00	26.17	B	
ATOM	2687	O	ARG	26	49.965	-2.367	55.500	1.00	27.47	B	
ATOM	2688	N	PRO	27	50.296	-0.748	53.976	1.00	28.46	B	
ATOM	2689	CD	PRO	27	49.815	0.221	52.972	1.00	28.96	B	
ATOM	2690	CA	PRO	27	51.634	-1.225	53.617	1.00	30.05	B	
ATOM	2691	CB	PRO	27	51.757	-0.791	52.157	1.00	29.21	B	
ATOM	2692	CG	PRO	27	51.081	0.508	52.153	1.00	27.78	B	
ATOM	2693	C	PRO	27	52.652	-0.565	54.551	1.00	30.74	B	
ATOM	2694	O	PRO	27	52.315	0.387	55.255	1.00	30.33	B	
ATOM	2695	N	PHE	28	53.888	-1.065	54.559	1.00	33.00	B	
ATOM	2696	CA	PHE	28	54.946	-0.488	55.397	1.00	35.47	B	
ATOM	2697	CB	PHE	28	56.197	-1.349	55.423	1.00	34.78	B	
ATOM	2698	CG	PHE	28	56.043	-2.621	56.180	1.00	34.30	B	
ATOM	2699	CD1	PHE	28	55.970	-3.848	55.506	1.00	33.11	B	
ATOM	2700	CD2	PHE	28	55.975	-2.598	57.566	1.00	34.50	B	
ATOM	2701	CE1	PHE	28	55.831	-5.030	56.204	1.00	32.04	B	
ATOM	2702	CE2	PHE	28	55.833	-3.779	58.283	1.00	34.83	B	
ATOM	2703	CZ	PHE	28	55.762	-5.002	57.594	1.00	34.76	B	
ATOM	2704	C	PHE	28	55.432	0.848	54.837	1.00	37.44	B	
ATOM	2705	O	PHE	28	55.529	1.019	53.640	1.00	37.96	B	
ATOM	2706	N	ASN	29	55.724	1.797	55.719	1.00	41.21	B	
ATOM	2707	CA	ASN	29	56.195	3.114	55.288	1.00	43.97	B	
ATOM	2708	CB	ASN	29	55.731	4.190	56.280	1.00	42.30	B	
ATOM	2709	CG	ASN	29	56.080	3.843	57.724	1.00	41.84	B	
ATOM	2710	OD1	ASN	29	57.230	3.554	58.038	1.00	40.87	B	
ATOM	2711	ND2	ASN	29	55.080	3.866	58.604	1.00	40.16	B	
ATOM	2712	C	ASN	29	57.718	3.112	55.190	1.00	47.03	B	
ATOM	2713	O	ASN	29	58.361	2.179	55.651	1.00	48.57	B	
ATOM	2714	N	LEU	30	58.290	4.156	54.594	1.00	49.85	B	
ATOM	2715	CA	LEU	30	59.745	4.258	54.442	1.00	52.56	B	
ATOM	2716	CB	LEU	30	60.125	5.641	53.928	1.00	52.63	B	
ATOM	2717	CG	LEU	30	60.214	5.735	52.409	1.00	53.20	B	
ATOM	2718	CD1	LEU	30	60.395	7.194	51.973	1.00	53.18	B	
ATOM	2719	CD2	LEU	30	61.378	4.862	51.935	1.00	54.30	B	
ATOM	2720	C	LEU	30	60.579	3.978	55.695	1.00	54.36	B	
ATOM	2721	O	LEU	30	61.623	3.347	55.619	1.00	54.97	B	
ATOM	2722	N	ALA	31	60.121	4.453	56.847	1.00	56.36	B	
ATOM	2723	CA	ALA	31	60.843	4.228	58.097	1.00	58.76	B	
ATOM	2724	CB	ALA	31	60.214	5.057	59.202	1.00	58.55	B	
ATOM	2725	C	ALA	31	60.842	2.742	58.487	1.00	60.40	B	
ATOM	2726	O	ALA	31	61.749	2.266	59.167	1.00	60.67	B	
ATOM	2727	N	GLU	32	59.819	2.016	58.045	1.00	61.95	B	
ATOM	2728	CA	GLU	32	59.692	0.594	58.350	1.00	63.39	B	
ATOM	2729	CB	GLU	32	58.215	0.187	58.322	1.00	62.91	B	
ATOM	2730	CG	GLU	32	57.429	0.683	59.524	1.00	62.16	B	
ATOM	2731	CD	GLU	32	55.933	0.669	59.299	1.00	61.37	B	
ATOM	2732	OE1	GLU	32	55.191	0.841	60.289	1.00	60.97	B	
ATOM	2733	OE2	GLU	32	55.504	0.497	58.138	1.00	60.36	B	
ATOM	2734	C	GLU	32	60.487	-0.318	57.414	1.00	64.76	B	
ATOM	2735	O	GLU	32	61.130	-1.261	57.860	1.00	64.21	B	
ATOM	2736	N	ARG	33	60.436	-0.039	56.116	1.00	66.90	B	
ATOM	2737	CA	ARG	33	61.150	-0.855	55.141	1.00	69.19	B	
ATOM	2738	CB	ARG	33	60.690	-0.503	53.719	1.00	70.74	B	
ATOM	2739	CG	ARG	33	60.911	0.953	53.310	1.00	73.78	B	
ATOM	2740	CD	ARG	33	60.238	1.267	51.977	1.00	75.17	B	
ATOM	2741	NE	ARG	33	60.663	0.349	50.920	1.00	76.52	B	
ATOM	2742	CZ	ARG	33	61.889	0.301	50.400	1.00	76.92	B	
ATOM	2743	NH1	ARG	33	62.838	1.122	50.829	1.00	76.57	B	
ATOM	2744	NH2	ARG	33	62.168	-0.569	49.441	1.00	78.04	B	

ATOM	2745	C	ARG	33	62.650	-0.654	55.297	1.00	70.11	B
ATOM	2746	O	ARG	33	63.439	-1.524	54.943	1.00	70.36	B
ATOM	2747	N	LYS	34	63.038	0.500	55.832	1.00	71.13	B
ATOM	2748	CA	LYS	34	64.447	0.798	56.053	1.00	72.18	B
ATOM	2749	CB	LYS	34	64.623	2.254	56.498	1.00	73.21	B
ATOM	2750	CG	LYS	34	64.611	3.267	55.363	1.00	74.27	B
ATOM	2751	CD	LYS	34	66.023	3.637	54.921	1.00	74.99	B
ATOM	2752	CE	LYS	34	66.769	2.463	54.306	1.00	74.88	B
ATOM	2753	NZ	LYS	34	68.154	2.852	53.916	1.00	75.81	B
ATOM	2754	C	LYS	34	65.006	-0.137	57.123	1.00	72.12	B
ATOM	2755	O	LYS	34	66.207	-0.424	57.142	1.00	72.82	B
ATOM	2756	N	ALA	35	64.130	-0.612	58.007	1.00	71.37	B
ATOM	2757	CA	ALA	35	64.522	-1.526	59.077	1.00	69.94	B
ATOM	2758	CB	ALA	35	63.780	-1.177	60.361	1.00	69.77	B
ATOM	2759	C	ALA	35	64.223	-2.970	58.685	1.00	69.24	B
ATOM	2760	O	ALA	35	64.198	-3.854	59.542	1.00	69.32	B
ATOM	2761	N	SER	36	64.001	-3.194	57.388	1.00	68.43	B
ATOM	2762	CA	SER	36	63.689	-4.519	56.848	1.00	66.99	B
ATOM	2763	CB	SER	36	64.937	-5.405	56.860	1.00	67.27	B
ATOM	2764	OG	SER	36	65.906	-4.912	55.959	1.00	67.40	B
ATOM	2765	C	SER	36	62.579	-5.159	57.674	1.00	65.70	B
ATOM	2766	O	SER	36	62.721	-6.270	58.185	1.00	65.65	B
ATOM	2767	N	ALA	37	61.469	-4.435	57.791	1.00	64.41	B
ATOM	2768	CA	ALA	37	60.320	-4.880	58.568	1.00	62.00	B
ATOM	2769	CB	ALA	37	59.256	-3.784	58.601	1.00	62.35	B
ATOM	2770	C	ALA	37	59.699	-6.185	58.093	1.00	59.79	B
ATOM	2771	O	ALA	37	59.490	-6.404	56.909	1.00	58.90	B
ATOM	2772	N	HIS	38	59.400	-7.042	59.061	1.00	58.16	B
ATOM	2773	CA	HIS	38	58.795	-8.347	58.828	1.00	55.57	B
ATOM	2774	CB	HIS	38	59.420	-9.381	59.785	1.00	57.59	B
ATOM	2775	CG	HIS	38	59.426	-8.963	61.233	1.00	58.97	B
ATOM	2776	CD2	HIS	38	58.878	-9.543	62.328	1.00	58.78	B
ATOM	2777	ND1	HIS	38	60.083	-7.837	61.689	1.00	58.86	B
ATOM	2778	CE1	HIS	38	59.939	-7.744	63.000	1.00	58.84	B
ATOM	2779	NE2	HIS	38	59.211	-8.766	63.412	1.00	58.91	B
ATOM	2780	C	HIS	38	57.296	-8.223	59.086	1.00	53.05	B
ATOM	2781	O	HIS	38	56.890	-7.787	60.163	1.00	54.10	B
ATOM	2782	N	SER	39	56.472	-8.605	58.114	1.00	48.25	B
ATOM	2783	CA	SER	39	55.026	-8.500	58.290	1.00	42.98	B
ATOM	2784	CB	SER	39	54.295	-8.575	56.970	1.00	42.55	B
ATOM	2785	OG	SER	39	52.903	-8.490	57.201	1.00	39.13	B
ATOM	2786	C	SER	39	54.444	-9.616	59.130	1.00	40.52	B
ATOM	2787	O	SER	39	54.750	-10.773	58.919	1.00	39.58	B
ATOM	2788	N	ILE	40	53.603	-9.247	60.092	1.00	38.79	B
ATOM	2789	CA	ILE	40	52.967	-10.222	60.979	1.00	36.32	B
ATOM	2790	CB	ILE	40	53.039	-9.786	62.478	1.00	37.00	B
ATOM	2791	CG2	ILE	40	54.493	-9.677	62.925	1.00	37.72	B
ATOM	2792	CG1	ILE	40	52.307	-8.458	62.692	1.00	37.68	B
ATOM	2793	CD1	ILE	40	52.102	-8.097	64.161	1.00	37.35	B
ATOM	2794	C	ILE	40	51.501	-10.426	60.611	1.00	34.00	B
ATOM	2795	O	ILE	40	50.757	-11.084	61.319	1.00	32.93	B
ATOM	2796	N	VAL	41	51.097	-9.863	59.482	1.00	33.39	B
ATOM	2797	CA	VAL	41	49.720	-9.986	59.028	1.00	32.21	B
ATOM	2798	CB	VAL	41	48.982	-8.617	59.042	1.00	31.99	B
ATOM	2799	CG1	VAL	41	47.559	-8.778	58.536	1.00	30.52	B
ATOM	2800	CG2	VAL	41	48.964	-8.048	60.445	1.00	32.73	B
ATOM	2801	C	VAL	41	49.685	-10.526	57.610	1.00	32.35	B
ATOM	2802	O	VAL	41	50.357	-10.022	56.728	1.00	31.91	B
ATOM	2803	N	GLU	42	48.886	-11.565	57.417	1.00	33.52	B
ATOM	2804	CA	GLU	42	48.727	-12.189	56.112	1.00	34.79	B
ATOM	2805	CB	GLU	42	49.228	-13.626	56.142	1.00	34.88	B
ATOM	2806	CG	GLU	42	50.715	-13.762	55.882	1.00	35.91	B
ATOM	2807	CD	GLU	42	51.222	-15.139	56.222	1.00	36.62	B
ATOM	2808	OE1	GLU	42	50.467	-16.105	55.996	1.00	35.55	B
ATOM	2809	OE2	GLU	42	52.373	-15.262	56.704	1.00	36.67	B
ATOM	2810	C	GLU	42	47.264	-12.207	55.689	1.00	34.67	B
ATOM	2811	O	GLU	42	46.425	-12.745	56.388	1.00	35.11	B
ATOM	2812	N	CYS	43	46.959	-11.615	54.540	1.00	33.53	B
ATOM	2813	CA	CYS	43	45.581	-11.575	54.074	1.00	33.64	B
ATOM	2814	CB	CYS	43	45.241	-10.172	53.575	1.00	31.73	B
ATOM	2815	SG	CYS	43	45.291	-8.913	54.863	1.00	30.24	B
ATOM	2816	C	CYS	43	45.306	-12.597	52.985	1.00	34.68	B
ATOM	2817	O	CYS	43	46.052	-12.722	52.025	1.00	35.47	B

ATOM	2818	N	ASP	44	44.220	-13.335	53.160	1.00	34.51	B
ATOM	2819	CA	ASP	44	43.821	-14.347	52.196	1.00	35.72	B
ATOM	2820	CB	ASP	44	43.698	-15.710	52.875	1.00	37.74	B
ATOM	2821	CG	ASP	44	43.627	-16.858	51.880	1.00	39.14	B
ATOM	2822	OD1	ASP	44	43.029	-16.681	50.787	1.00	38.15	B
ATOM	2823	OD2	ASP	44	44.166	-17.941	52.206	1.00	40.23	B
ATOM	2824	C	ASP	44	42.452	-13.949	51.662	1.00	36.02	B
ATOM	2825	O	ASP	44	41.433	-14.323	52.228	1.00	34.41	B
ATOM	2826	N	PRO	45	42.415	-13.177	50.566	1.00	36.48	B
ATOM	2827	CD	PRO	45	43.558	-12.792	49.725	1.00	37.08	B
ATOM	2828	CA	PRO	45	41.162	-12.727	49.962	1.00	36.44	B
ATOM	2829	CB	PRO	45	41.646	-11.834	48.828	1.00	36.90	B
ATOM	2830	CG	PRO	45	42.892	-12.518	48.398	1.00	37.61	B
ATOM	2831	C	PRO	45	40.254	-13.872	49.518	1.00	36.95	B
ATOM	2832	O	PRO	45	39.046	-13.805	49.685	1.00	37.27	B
ATOM	2833	N	VAL	46	40.834	-14.912	48.930	1.00	37.39	B
ATOM	2834	CA	VAL	46	40.051	-16.057	48.479	1.00	37.62	B
ATOM	2835	CB	VAL	46	40.943	-17.087	47.773	1.00	38.49	B
ATOM	2836	CG1	VAL	46	40.099	-18.269	47.334	1.00	39.31	B
ATOM	2837	CG2	VAL	46	41.642	-16.436	46.584	1.00	38.33	B
ATOM	2838	C	VAL	46	39.354	-16.728	49.665	1.00	37.65	B
ATOM	2839	O	VAL	46	38.172	-17.082	49.606	1.00	38.03	B
ATOM	2840	N	ARG	47	40.089	-16.902	50.752	1.00	37.10	B
ATOM	2841	CA	ARG	47	39.520	-17.512	51.947	1.00	37.76	B
ATOM	2842	CB	ARG	47	40.627	-18.142	52.797	1.00	40.98	B
ATOM	2843	CG	ARG	47	40.138	-19.170	53.811	1.00	45.53	B
ATOM	2844	CD	ARG	47	40.088	-20.569	53.205	1.00	48.08	B
ATOM	2845	NE	ARG	47	41.427	-21.065	52.905	1.00	51.05	B
ATOM	2846	CZ	ARG	47	42.361	-21.291	53.826	1.00	53.04	B
ATOM	2847	NH1	ARG	47	42.101	-21.066	55.108	1.00	53.32	B
ATOM	2848	NH2	ARG	47	43.558	-21.744	53.467	1.00	53.55	B
ATOM	2849	C	ARG	47	38.817	-16.436	52.774	1.00	35.87	B
ATOM	2850	O	ARG	47	38.091	-16.734	53.702	1.00	35.14	B
ATOM	2851	N	LYS	48	39.054	-15.178	52.420	1.00	34.57	B
ATOM	2852	CA	LYS	48	38.456	-14.051	53.125	1.00	32.91	B
ATOM	2853	CB	LYS	48	36.938	-14.158	53.092	1.00	34.16	B
ATOM	2854	CG	LYS	48	36.361	-14.145	51.693	1.00	36.73	B
ATOM	2855	CD	LYS	48	34.854	-14.249	51.706	1.00	37.41	B
ATOM	2856	CE	LYS	48	34.338	-14.550	50.314	1.00	38.70	B
ATOM	2857	NZ	LYS	48	34.704	-13.479	49.344	1.00	36.20	B
ATOM	2858	C	LYS	48	38.903	-13.978	54.578	1.00	31.33	B
ATOM	2859	O	LYS	48	38.140	-13.593	55.440	1.00	31.50	B
ATOM	2860	N	GLU	49	40.151	-14.352	54.836	1.00	29.95	B
ATOM	2861	CA	GLU	49	40.692	-14.330	56.193	1.00	27.26	B
ATOM	2862	CB	GLU	49	41.168	-15.719	56.633	1.00	28.44	B
ATOM	2863	CG	GLU	49	40.135	-16.815	56.656	1.00	28.64	B
ATOM	2864	CD	GLU	49	40.760	-18.160	56.980	1.00	29.46	B
ATOM	2865	OE1	GLU	49	40.028	-19.168	56.992	1.00	29.37	B
ATOM	2866	OE2	GLU	49	41.986	-18.211	57.220	1.00	29.95	B
ATOM	2867	C	GLU	49	41.924	-13.438	56.344	1.00	24.62	B
ATOM	2868	O	GLU	49	42.648	-13.164	55.395	1.00	23.41	B
ATOM	2869	N	VAL	50	42.123	-12.973	57.565	1.00	23.85	B
ATOM	2870	CA	VAL	50	43.276	-12.164	57.915	1.00	22.58	B
ATOM	2871	CB	VAL	50	42.852	-10.738	58.417	1.00	21.03	B
ATOM	2872	CG1	VAL	50	41.863	-10.851	59.540	1.00	20.58	B
ATOM	2873	CG2	VAL	50	44.047	-9.968	58.884	1.00	19.55	B
ATOM	2874	C	VAL	50	43.909	-12.995	59.036	1.00	23.21	B
ATOM	2875	O	VAL	50	43.234	-13.410	59.959	1.00	22.47	B
ATOM	2876	N	SER	51	45.197	-13.286	58.923	1.00	24.22	B
ATOM	2877	CA	SER	51	45.867	-14.078	59.950	1.00	26.05	B
ATOM	2878	CB	SER	51	46.398	-15.380	59.352	1.00	26.43	B
ATOM	2879	OG	SER	51	46.705	-16.299	60.383	1.00	26.88	B
ATOM	2880	C	SER	51	47.013	-13.293	60.579	1.00	26.62	B
ATOM	2881	O	SER	51	47.893	-12.781	59.868	1.00	26.40	B
ATOM	2882	N	VAL	52	46.998	-13.213	61.908	1.00	27.16	B
ATOM	2883	CA	VAL	52	48.000	-12.463	62.657	1.00	29.10	B
ATOM	2884	CB	VAL	52	47.311	-11.480	63.640	1.00	28.02	B
ATOM	2885	CG1	VAL	52	48.336	-10.624	64.340	1.00	27.20	B
ATOM	2886	CG2	VAL	52	46.341	-10.607	62.885	1.00	27.34	B
ATOM	2887	C	VAL	52	48.974	-13.331	63.442	1.00	30.28	B
ATOM	2888	O	VAL	52	48.567	-14.267	64.117	1.00	30.72	B
ATOM	2889	N	ARG	53	50.265	-13.018	63.342	1.00	31.46	B
ATOM	2890	CA	ARG	53	51.276	-13.778	64.070	1.00	32.95	B

ATOM	2891	CB	ARG	53	52.615	-13.750	63.336	1.00	33.14	B
ATOM	2892	CG	ARG	53	53.636	-14.706	63.926	1.00	32.63	B
ATOM	2893	CD	ARG	53	54.575	-15.197	62.851	1.00	33.53	B
ATOM	2894	NE	ARG	53	55.482	-14.163	62.378	1.00	34.35	B
ATOM	2895	CZ	ARG	53	56.017	-14.140	61.161	1.00	35.36	B
ATOM	2896	NH1	ARG	53	55.738	-15.089	60.272	1.00	35.11	B
ATOM	2897	NH2	ARG	53	56.847	-13.162	60.838	1.00	36.70	B
ATOM	2898	C	ARG	53	51.423	-13.182	65.458	1.00	34.27	B
ATOM	2899	O	ARG	53	51.964	-12.088	65.632	1.00	34.80	B
ATOM	2900	N	THR	54	50.931	-13.915	66.446	1.00	35.04	B
ATOM	2901	CA	THR	54	50.977	-13.458	67.815	1.00	37.72	B
ATOM	2902	CB	THR	54	49.672	-13.823	68.540	1.00	37.47	B
ATOM	2903	OG1	THR	54	49.521	-15.244	68.581	1.00	36.02	B
ATOM	2904	CG2	THR	54	48.484	-13.260	67.804	1.00	37.61	B
ATOM	2905	C	THR	54	52.141	-14.056	68.586	1.00	39.85	B
ATOM	2906	O	THR	54	52.517	-13.554	69.633	1.00	39.10	B
ATOM	2907	N	GLY	55	52.721	-15.121	68.043	1.00	43.17	B
ATOM	2908	CA	GLY	55	53.810	-15.791	68.727	1.00	48.23	B
ATOM	2909	C	GLY	55	55.214	-15.667	68.165	1.00	51.61	B
ATOM	2910	O	GLY	55	55.704	-14.562	67.926	1.00	52.45	B
ATOM	2911	N	GLY	56	55.855	-16.820	67.962	1.00	53.22	B
ATOM	2912	CA	GLY	56	57.219	-16.864	67.464	1.00	54.95	B
ATOM	2913	C	GLY	56	57.420	-16.365	66.052	1.00	56.66	B
ATOM	2914	O	GLY	56	56.733	-15.450	65.611	1.00	57.44	B
ATOM	2915	N	LEU	57	58.366	-16.980	65.346	1.00	57.72	B
ATOM	2916	CA	LEU	57	58.693	-16.600	63.972	1.00	58.30	B
ATOM	2917	CB	LEU	57	60.219	-16.608	63.777	1.00	58.78	B
ATOM	2918	CG	LEU	57	61.067	-17.384	64.790	1.00	59.20	B
ATOM	2919	CD1	LEU	57	60.709	-18.870	64.762	1.00	59.75	B
ATOM	2920	CD2	LEU	57	62.542	-17.175	64.472	1.00	59.20	B
ATOM	2921	C	LEU	57	58.029	-17.493	62.921	1.00	58.10	B
ATOM	2922	O	LEU	57	57.153	-18.289	63.245	1.00	58.57	B
ATOM	2923	N	ALA	58	58.450	-17.343	61.665	1.00	57.02	B
ATOM	2924	CA	ALA	58	57.905	-18.126	60.555	1.00	55.81	B
ATOM	2925	CB	ALA	58	58.473	-17.615	59.235	1.00	55.75	B
ATOM	2926	C	ALA	58	58.193	-19.622	60.705	1.00	54.88	B
ATOM	2927	O	ALA	58	57.350	-20.460	60.375	1.00	54.40	B
ATOM	2928	N	ASP	59	59.386	-19.937	61.211	1.00	53.60	B
ATOM	2929	CA	ASP	59	59.845	-21.316	61.431	1.00	51.49	B
ATOM	2930	CB	ASP	59	61.254	-21.290	62.050	1.00	51.99	B
ATOM	2931	CG	ASP	59	61.807	-22.681	62.338	1.00	52.10	B
ATOM	2932	OD1	ASP	59	62.005	-23.464	61.385	1.00	51.56	B
ATOM	2933	OD2	ASP	59	62.051	-22.987	63.525	1.00	52.60	B
ATOM	2934	C	ASP	59	58.903	-22.110	62.338	1.00	49.40	B
ATOM	2935	O	ASP	59	58.742	-23.315	62.197	1.00	48.84	B
ATOM	2936	N	LYS	60	58.267	-21.404	63.256	1.00	47.59	B
ATOM	2937	CA	LYS	60	57.366	-22.021	64.208	1.00	46.47	B
ATOM	2938	CB	LYS	60	58.178	-22.949	65.114	1.00	45.88	B
ATOM	2939	CG	LYS	60	57.465	-23.470	66.345	1.00	44.88	B
ATOM	2940	CD	LYS	60	58.462	-24.217	67.209	1.00	45.79	B
ATOM	2941	CE	LYS	60	57.868	-24.729	68.503	1.00	47.18	B
ATOM	2942	NZ	LYS	60	58.938	-25.298	69.384	1.00	48.54	B
ATOM	2943	C	LYS	60	56.745	-20.862	64.977	1.00	45.74	B
ATOM	2944	O	LYS	60	57.468	-20.017	65.532	1.00	45.66	B
ATOM	2945	N	SER	61	55.417	-20.802	64.999	1.00	44.14	B
ATOM	2946	CA	SER	61	54.750	-19.718	65.697	1.00	42.32	B
ATOM	2947	CB	SER	61	54.900	-18.419	64.892	1.00	43.45	B
ATOM	2948	OG	SER	61	54.484	-18.594	63.545	1.00	42.02	B
ATOM	2949	C	SER	61	53.267	-19.931	65.980	1.00	40.98	B
ATOM	2950	O	SER	61	52.679	-20.939	65.613	1.00	40.30	B
ATOM	2951	N	SER	62	52.686	-18.954	66.669	1.00	40.63	B
ATOM	2952	CA	SER	62	51.265	-18.944	66.992	1.00	38.79	B
ATOM	2953	CB	SER	62	51.032	-18.549	68.445	1.00	38.80	B
ATOM	2954	OG	SER	62	51.678	-19.441	69.325	1.00	38.30	B
ATOM	2955	C	SER	62	50.634	-17.862	66.115	1.00	37.30	B
ATOM	2956	O	SER	62	51.293	-16.906	65.728	1.00	37.14	B
ATOM	2957	N	ARG	63	49.361	-18.018	65.783	1.00	36.69	B
ATOM	2958	CA	ARG	63	48.687	-17.017	64.959	1.00	35.86	B
ATOM	2959	CB	ARG	63	48.827	-17.318	63.453	1.00	35.76	B
ATOM	2960	CG	ARG	63	50.264	-17.378	62.918	1.00	36.93	B
ATOM	2961	CD	ARG	63	50.303	-17.660	61.418	1.00	38.47	B
ATOM	2962	NE	ARG	63	49.917	-16.499	60.608	1.00	40.73	B
ATOM	2963	CZ	ARG	63	50.685	-15.428	60.393	1.00	40.83	B

ATOM	2964	NH1	ARG	63	51.896	-15.353	60.928	1.00	41.75	B
ATOM	2965	NH2	ARG	63	50.250	-14.433	59.629	1.00	40.58	B
ATOM	2966	C	ARG	63	47.206	-16.982	65.296	1.00	34.60	B
ATOM	2967	O	ARG	63	46.656	-17.920	65.855	1.00	33.92	B
ATOM	2968	N	LYS	64	46.578	-15.865	64.968	1.00	33.48	B
ATOM	2969	CA	LYS	64	45.158	-15.676	65.193	1.00	31.00	B
ATOM	2970	CB	LYS	64	44.913	-14.444	66.056	1.00	34.47	B
ATOM	2971	CG	LYS	64	45.324	-14.581	67.508	1.00	36.74	B
ATOM	2972	CD	LYS	64	44.298	-15.378	68.279	1.00	38.57	B
ATOM	2973	CE	LYS	64	44.593	-15.324	69.773	1.00	39.71	B
ATOM	2974	NZ	LYS	64	43.520	-15.964	70.596	1.00	40.02	B
ATOM	2975	C	LYS	64	44.592	-15.428	63.805	1.00	29.35	B
ATOM	2976	O	LYS	64	45.114	-14.604	63.045	1.00	29.23	B
ATOM	2977	N	THR	65	43.537	-16.156	63.470	1.00	27.29	B
ATOM	2978	CA	THR	65	42.917	-16.020	62.165	1.00	24.96	B
ATOM	2979	CB	THR	65	43.062	-17.321	61.338	1.00	24.86	B
ATOM	2980	OG1	THR	65	44.442	-17.701	61.294	1.00	24.93	B
ATOM	2981	CG2	THR	65	42.555	-17.120	59.912	1.00	25.70	B
ATOM	2982	C	THR	65	41.449	-15.688	62.319	1.00	22.74	B
ATOM	2983	O	THR	65	40.752	-16.313	63.095	1.00	23.83	B
ATOM	2984	N	TYR	66	40.999	-14.677	61.579	1.00	21.85	B
ATOM	2985	CA	TYR	66	39.601	-14.232	61.612	1.00	20.45	B
ATOM	2986	CB	TYR	66	39.480	-12.844	62.234	1.00	18.74	B
ATOM	2987	CG	TYR	66	40.144	-12.695	63.581	1.00	19.02	B
ATOM	2988	CD1	TYR	66	41.524	-12.584	63.695	1.00	18.23	B
ATOM	2989	CE1	TYR	66	42.136	-12.420	64.946	1.00	19.22	B
ATOM	2990	CD2	TYR	66	39.387	-12.641	64.748	1.00	20.12	B
ATOM	2991	CE2	TYR	66	39.986	-12.474	66.009	1.00	19.66	B
ATOM	2992	CZ	TYR	66	41.357	-12.367	66.109	1.00	20.40	B
ATOM	2993	OH	TYR	66	41.915	-12.234	67.382	1.00	20.35	B
ATOM	2994	C	TYR	66	39.027	-14.136	60.195	1.00	22.62	B
ATOM	2995	O	TYR	66	39.736	-13.786	59.237	1.00	22.83	B
ATOM	2996	N	THR	67	37.747	-14.464	60.058	1.00	22.62	B
ATOM	2997	CA	THR	67	37.099	-14.424	58.755	1.00	23.36	B
ATOM	2998	CB	THR	67	36.299	-15.723	58.489	1.00	24.24	B
ATOM	2999	OG1	THR	67	37.169	-16.854	58.576	1.00	26.83	B
ATOM	3000	CG2	THR	67	35.679	-15.702	57.115	1.00	25.09	B
ATOM	3001	C	THR	67	36.145	-13.241	58.669	1.00	23.25	B
ATOM	3002	O	THR	67	35.383	-12.979	59.598	1.00	23.74	B
ATOM	3003	N	PHE	68	36.199	-12.521	57.556	1.00	22.27	B
ATOM	3004	CA	PHE	68	35.322	-11.379	57.354	1.00	23.47	B
ATOM	3005	CB	PHE	68	36.108	-10.068	57.414	1.00	25.18	B
ATOM	3006	CG	PHE	68	36.688	-9.788	58.758	1.00	28.91	B
ATOM	3007	CD1	PHE	68	37.872	-10.407	59.162	1.00	31.76	B
ATOM	3008	CD2	PHE	68	36.028	-8.957	59.655	1.00	30.45	B
ATOM	3009	CE1	PHE	68	38.397	-10.211	60.444	1.00	33.13	B
ATOM	3010	CE2	PHE	68	36.539	-8.749	60.947	1.00	32.68	B
ATOM	3011	CZ	PHE	68	37.733	-9.381	61.346	1.00	34.40	B
ATOM	3012	C	PHE	68	34.664	-11.530	56.001	1.00	23.18	B
ATOM	3013	O	PHE	68	34.904	-12.505	55.318	1.00	23.09	B
ATOM	3014	N	ASP	69	33.836	-10.560	55.625	1.00	22.35	B
ATOM	3015	CA	ASP	69	33.127	-10.585	54.350	1.00	23.38	B
ATOM	3016	CB	ASP	69	31.988	-9.559	54.386	1.00	23.05	B
ATOM	3017	CG	ASP	69	30.917	-9.915	55.427	1.00	23.94	B
ATOM	3018	OD1	ASP	69	30.875	-9.341	56.538	1.00	21.68	B
ATOM	3019	OD2	ASP	69	30.106	-10.812	55.138	1.00	25.46	B
ATOM	3020	C	ASP	69	34.071	-10.363	53.173	1.00	24.90	B
ATOM	3021	O	ASP	69	33.880	-10.931	52.082	1.00	25.83	B
ATOM	3022	N	MET	70	35.089	-9.539	53.405	1.00	25.78	B
ATOM	3023	CA	MET	70	36.112	-9.233	52.412	1.00	26.18	B
ATOM	3024	CB	MET	70	35.686	-8.073	51.517	1.00	27.89	B
ATOM	3025	CG	MET	70	34.538	-8.363	50.564	1.00	29.68	B
ATOM	3026	SD	MET	70	34.155	-6.927	49.495	1.00	34.95	B
ATOM	3027	CE	MET	70	32.418	-7.227	49.126	1.00	32.58	B
ATOM	3028	C	MET	70	37.378	-8.801	53.150	1.00	25.52	B
ATOM	3029	O	MET	70	37.301	-8.187	54.206	1.00	26.04	B
ATOM	3030	N	VAL	71	38.540	-9.119	52.596	1.00	24.01	B
ATOM	3031	CA	VAL	71	39.789	-8.724	53.228	1.00	23.48	B
ATOM	3032	CB	VAL	71	40.496	-9.917	53.902	1.00	24.24	B
ATOM	3033	CG1	VAL	71	39.668	-10.429	55.086	1.00	23.32	B
ATOM	3034	CG2	VAL	71	40.726	-11.004	52.882	1.00	24.53	B
ATOM	3035	C	VAL	71	40.709	-8.121	52.181	1.00	23.86	B
ATOM	3036	O	VAL	71	40.841	-8.641	51.068	1.00	22.79	B

ATOM	3037	N	PHE	72	41.356	-7.025	52.551	1.00	22.62	B
ATOM	3038	CA	PHE	72	42.229	-6.344	51.628	1.00	22.70	B
ATOM	3039	CB	PHE	72	41.710	-4.936	51.321	1.00	20.63	B
ATOM	3040	CG	PHE	72	40.318	-4.910	50.753	1.00	18.35	B
ATOM	3041	CD1	PHE	72	40.056	-5.419	49.493	1.00	15.95	B
ATOM	3042	CD2	PHE	72	39.261	-4.409	51.495	1.00	17.50	B
ATOM	3043	CE1	PHE	72	38.771	-5.435	48.986	1.00	16.14	B
ATOM	3044	CE2	PHE	72	37.976	-4.425	50.985	1.00	17.48	B
ATOM	3045	CZ	PHE	72	37.732	-4.939	49.729	1.00	16.21	B
ATOM	3046	C	PHE	72	43.626	-6.197	52.178	1.00	22.69	B
ATOM	3047	O	PHE	72	43.836	-5.523	53.181	1.00	22.50	B
ATOM	3048	N	GLY	73	44.578	-6.837	51.508	1.00	22.82	B
ATOM	3049	CA	GLY	73	45.965	-6.741	51.920	1.00	23.34	B
ATOM	3050	C	GLY	73	46.584	-5.398	51.571	1.00	23.29	B
ATOM	3051	O	GLY	73	45.982	-4.561	50.885	1.00	22.64	B
ATOM	3052	N	ALA	74	47.809	-5.199	52.037	1.00	23.40	B
ATOM	3053	CA	ALA	74	48.531	-3.960	51.808	1.00	25.70	B
ATOM	3054	CB	ALA	74	49.891	-4.016	52.523	1.00	25.78	B
ATOM	3055	C	ALA	74	48.725	-3.639	50.328	1.00	26.16	B
ATOM	3056	O	ALA	74	49.129	-2.556	49.978	1.00	27.50	B
ATOM	3057	N	SER	75	48.406	-4.584	49.459	1.00	27.00	B
ATOM	3058	CA	SER	75	48.590	-4.358	48.031	1.00	28.47	B
ATOM	3059	CB	SER	75	48.982	-5.679	47.335	1.00	28.85	B
ATOM	3060	OG	SER	75	48.019	-6.709	47.507	1.00	27.19	B
ATOM	3061	C	SER	75	47.389	-3.728	47.319	1.00	27.90	B
ATOM	3062	O	SER	75	47.542	-3.123	46.243	1.00	29.21	B
ATOM	3063	N	THR	76	46.206	-3.853	47.918	1.00	26.99	B
ATOM	3064	CA	THR	76	44.984	-3.315	47.320	1.00	25.45	B
ATOM	3065	CB	THR	76	43.746	-3.663	48.183	1.00	23.54	B
ATOM	3066	OG1	THR	76	44.015	-3.345	49.545	1.00	23.44	B
ATOM	3067	CG2	THR	76	43.436	-5.132	48.116	1.00	24.38	B
ATOM	3068	C	THR	76	45.034	-1.803	47.087	1.00	25.69	B
ATOM	3069	O	THR	76	45.543	-1.041	47.922	1.00	27.74	B
ATOM	3070	N	LYS	77	44.507	-1.372	45.948	1.00	24.67	B
ATOM	3071	CA	LYS	77	44.496	0.044	45.619	1.00	23.51	B
ATOM	3072	CB	LYS	77	44.804	0.234	44.133	1.00	25.56	B
ATOM	3073	CG	LYS	77	46.192	-0.249	43.719	1.00	28.23	B
ATOM	3074	CD	LYS	77	46.373	-0.132	42.209	1.00	31.78	B
ATOM	3075	CE	LYS	77	47.770	-0.560	41.784	1.00	33.69	B
ATOM	3076	NZ	LYS	77	47.942	-0.449	40.311	1.00	35.35	B
ATOM	3077	C	LYS	77	43.150	0.677	45.956	1.00	21.23	B
ATOM	3078	O	LYS	77	42.175	-0.023	46.154	1.00	19.65	B
ATOM	3079	N	GLN	78	43.105	2.008	46.021	1.00	20.16	B
ATOM	3080	CA	GLN	78	41.853	2.714	46.335	1.00	18.91	B
ATOM	3081	CB	GLN	78	42.004	4.226	46.179	1.00	18.69	B
ATOM	3082	CG	GLN	78	43.063	4.851	47.064	1.00	18.42	B
ATOM	3083	CD	GLN	78	42.618	4.962	48.498	1.00	17.41	B
ATOM	3084	OE1	GLN	78	42.152	3.997	49.085	1.00	20.11	B
ATOM	3085	NE2	GLN	78	42.756	6.143	49.066	1.00	14.62	B
ATOM	3086	C	GLN	78	40.743	2.294	45.377	1.00	19.40	B
ATOM	3087	O	GLN	78	39.609	2.059	45.788	1.00	20.13	B
ATOM	3088	N	ILE	79	41.074	2.208	44.092	1.00	17.68	B
ATOM	3089	CA	ILE	79	40.089	1.815	43.094	1.00	15.86	B
ATOM	3090	CB	ILE	79	40.727	1.779	41.678	1.00	15.34	B
ATOM	3091	CG2	ILE	79	41.709	0.597	41.561	1.00	16.93	B
ATOM	3092	CG1	ILE	79	39.640	1.641	40.612	1.00	14.82	B
ATOM	3093	CD1	ILE	79	38.766	2.868	40.410	1.00	13.32	B
ATOM	3094	C	ILE	79	39.463	0.440	43.399	1.00	14.58	B
ATOM	3095	O	ILE	79	38.304	0.217	43.130	1.00	15.24	B
ATOM	3096	N	ASP	80	40.231	-0.479	43.969	1.00	13.09	B
ATOM	3097	CA	ASP	80	39.683	-1.802	44.258	1.00	12.77	B
ATOM	3098	CB	ASP	80	40.800	-2.818	44.435	1.00	14.43	B
ATOM	3099	CG	ASP	80	41.645	-2.953	43.204	1.00	18.24	B
ATOM	3100	OD1	ASP	80	41.072	-2.882	42.088	1.00	18.91	B
ATOM	3101	OD2	ASP	80	42.874	-3.140	43.363	1.00	21.75	B
ATOM	3102	C	ASP	80	38.787	-1.829	45.487	1.00	12.00	B
ATOM	3103	O	ASP	80	37.878	-2.638	45.590	1.00	10.17	B
ATOM	3104	N	VAL	81	39.063	-0.938	46.430	1.00	11.87	B
ATOM	3105	CA	VAL	81	38.261	-0.841	47.638	1.00	10.20	B
ATOM	3106	CB	VAL	81	38.881	0.128	48.642	1.00	9.09	B
ATOM	3107	CG1	VAL	81	37.857	0.529	49.689	1.00	7.52	B
ATOM	3108	CG2	VAL	81	40.071	-0.534	49.299	1.00	11.81	B
ATOM	3109	C	VAL	81	36.915	-0.292	47.224	1.00	10.85	B

ATOM	3110	O	VAL	81	35.879	-0.728	47.697	1.00	11.76	B
ATOM	3111	N	TYR	82	36.948	0.681	46.326	1.00	12.12	B
ATOM	3112	CA	TYR	82	35.735	1.304	45.845	1.00	13.85	B
ATOM	3113	CB	TYR	82	36.090	2.534	45.015	1.00	15.89	B
ATOM	3114	CG	TYR	82	34.870	3.259	44.530	1.00	18.66	B
ATOM	3115	CD1	TYR	82	34.364	3.029	43.256	1.00	20.38	B
ATOM	3116	CE1	TYR	82	33.201	3.645	42.824	1.00	22.59	B
ATOM	3117	CD2	TYR	82	34.184	4.132	45.369	1.00	19.71	B
ATOM	3118	CE2	TYR	82	33.019	4.755	44.953	1.00	22.44	B
ATOM	3119	CZ	TYR	82	32.531	4.508	43.675	1.00	23.44	B
ATOM	3120	OH	TYR	82	31.372	5.125	43.254	1.00	25.79	B
ATOM	3121	C	TYR	82	34.840	0.350	45.044	1.00	14.77	B
ATOM	3122	O	TYR	82	33.635	0.211	45.331	1.00	13.77	B
ATOM	3123	N	ARG	83	35.408	-0.299	44.035	1.00	15.58	B
ATOM	3124	CA	ARG	83	34.632	-1.236	43.220	1.00	18.14	B
ATOM	3125	CB	ARG	83	35.517	-1.815	42.103	1.00	20.58	B
ATOM	3126	CG	ARG	83	35.715	-0.868	40.915	1.00	23.85	B
ATOM	3127	CD	ARG	83	36.998	-1.162	40.161	1.00	26.52	B
ATOM	3128	NE	ARG	83	36.971	-2.428	39.436	1.00	30.77	B
ATOM	3129	CZ	ARG	83	36.255	-2.656	38.335	1.00	33.35	B
ATOM	3130	NH1	ARG	83	35.485	-1.703	37.818	1.00	33.79	B
ATOM	3131	NH2	ARG	83	36.339	-3.833	37.727	1.00	33.17	B
ATOM	3132	C	ARG	83	34.009	-2.382	44.045	1.00	18.55	B
ATOM	3133	O	ARG	83	32.867	-2.765	43.834	1.00	19.46	B
ATOM	3134	N	SER	84	34.764	-2.930	44.985	1.00	17.88	B
ATOM	3135	CA	SER	84	34.248	-4.009	45.809	1.00	17.71	B
ATOM	3136	CB	SER	84	35.380	-4.764	46.509	1.00	20.38	B
ATOM	3137	OG	SER	84	36.282	-5.324	45.575	1.00	25.36	B
ATOM	3138	C	SER	84	33.298	-3.551	46.913	1.00	16.07	B
ATOM	3139	O	SER	84	32.241	-4.113	47.073	1.00	15.35	B
ATOM	3140	N	VAL	85	33.685	-2.526	47.673	1.00	15.30	B
ATOM	3141	CA	VAL	85	32.865	-2.048	48.795	1.00	14.98	B
ATOM	3142	CB	VAL	85	33.738	-1.521	49.963	1.00	15.00	B
ATOM	3143	CG1	VAL	85	32.849	-1.183	51.129	1.00	15.00	B
ATOM	3144	CG2	VAL	85	34.775	-2.556	50.383	1.00	15.18	B
ATOM	3145	C	VAL	85	31.828	-0.960	48.509	1.00	14.85	B
ATOM	3146	O	VAL	85	30.652	-1.162	48.734	1.00	13.96	B
ATOM	3147	N	VAL	86	32.283	0.184	48.008	1.00	16.21	B
ATOM	3148	CA	VAL	86	31.409	1.313	47.740	1.00	15.47	B
ATOM	3149	CB	VAL	86	32.205	2.597	47.571	1.00	15.27	B
ATOM	3150	CG1	VAL	86	31.296	3.776	47.800	1.00	15.63	B
ATOM	3151	CG2	VAL	86	33.379	2.614	48.541	1.00	16.09	B
ATOM	3152	C	VAL	86	30.478	1.191	46.548	1.00	15.77	B
ATOM	3153	O	VAL	86	29.295	1.506	46.680	1.00	15.71	B
ATOM	3154	N	CYS	87	30.976	0.734	45.399	1.00	15.31	B
ATOM	3155	CA	CYS	87	30.121	0.629	44.218	1.00	17.14	B
ATOM	3156	CB	CYS	87	30.787	-0.168	43.108	1.00	16.23	B
ATOM	3157	SG	CYS	87	30.003	0.173	41.511	1.00	22.71	B
ATOM	3158	C	CYS	87	28.753	-0.001	44.488	1.00	18.54	B
ATOM	3159	O	CYS	87	27.752	0.494	44.050	1.00	19.06	B
ATOM	3160	N	PRO	88	28.707	-1.117	45.207	1.00	20.44	B
ATOM	3161	CD	PRO	88	29.827	-2.005	45.536	1.00	22.48	B
ATOM	3162	CA	PRO	88	27.422	-1.759	45.507	1.00	21.26	B
ATOM	3163	CB	PRO	88	27.847	-3.060	46.157	1.00	21.76	B
ATOM	3164	CG	PRO	88	29.168	-3.337	45.512	1.00	22.69	B
ATOM	3165	C	PRO	88	26.542	-0.890	46.434	1.00	22.59	B
ATOM	3166	O	PRO	88	25.333	-0.797	46.254	1.00	22.78	B
ATOM	3167	N	ILE	89	27.151	-0.273	47.446	1.00	22.51	B
ATOM	3168	CA	ILE	89	26.409	0.582	48.388	1.00	22.44	B
ATOM	3169	CB	ILE	89	27.298	1.003	49.579	1.00	22.87	B
ATOM	3170	CG2	ILE	89	26.592	2.040	50.408	1.00	22.27	B
ATOM	3171	CG1	ILE	89	27.607	-0.227	50.439	1.00	24.48	B
ATOM	3172	CD1	ILE	89	28.465	0.041	51.641	1.00	26.67	B
ATOM	3173	C	ILE	89	25.843	1.841	47.727	1.00	22.09	B
ATOM	3174	O	ILE	89	24.734	2.264	48.035	1.00	21.69	B
ATOM	3175	N	LEU	90	26.607	2.450	46.829	1.00	21.87	B
ATOM	3176	CA	LEU	90	26.122	3.640	46.157	1.00	23.17	B
ATOM	3177	CB	LEU	90	27.195	4.228	45.243	1.00	20.80	B
ATOM	3178	CG	LEU	90	26.773	5.485	44.498	1.00	18.97	B
ATOM	3179	CD1	LEU	90	26.169	6.492	45.446	1.00	18.16	B
ATOM	3180	CD2	LEU	90	27.987	6.053	43.822	1.00	20.13	B
ATOM	3181	C	LEU	90	24.891	3.282	45.334	1.00	24.49	B
ATOM	3182	O	LEU	90	23.963	4.091	45.207	1.00	24.70	B

ATOM	3183	N	ASP	91	24.887	2.068	44.781	1.00	25.50	B
ATOM	3184	CA	ASP	91	23.765	1.617	43.975	1.00	26.54	B
ATOM	3185	CB	ASP	91	24.042	0.258	43.331	1.00	27.25	B
ATOM	3186	CG	ASP	91	24.841	0.373	42.045	1.00	29.15	B
ATOM	3187	OD1	ASP	91	24.725	1.424	41.365	1.00	28.90	B
ATOM	3188	OD2	ASP	91	25.559	-0.601	41.701	1.00	29.60	B
ATOM	3189	C	ASP	91	22.537	1.512	44.848	1.00	27.48	B
ATOM	3190	O	ASP	91	21.427	1.740	44.399	1.00	28.35	B
ATOM	3191	N	GLU	92	22.736	1.185	46.115	1.00	28.27	B
ATOM	3192	CA	GLU	92	21.603	1.065	47.018	1.00	28.89	B
ATOM	3193	CB	GLU	92	22.008	0.214	48.219	1.00	30.33	B
ATOM	3194	CG	GLU	92	20.839	-0.266	49.057	1.00	33.34	B
ATOM	3195	CD	GLU	92	21.141	-1.578	49.772	1.00	35.27	B
ATOM	3196	OE1	GLU	92	20.340	-2.000	50.633	1.00	36.65	B
ATOM	3197	OE2	GLU	92	22.181	-2.200	49.469	1.00	35.05	B
ATOM	3198	C	GLU	92	21.106	2.459	47.424	1.00	28.34	B
ATOM	3199	O	GLU	92	19.897	2.685	47.581	1.00	27.53	B
ATOM	3200	N	VAL	93	22.037	3.395	47.585	1.00	27.17	B
ATOM	3201	CA	VAL	93	21.663	4.757	47.938	1.00	26.25	B
ATOM	3202	CB	VAL	93	22.902	5.681	48.072	1.00	27.41	B
ATOM	3203	CG1	VAL	93	22.455	7.125	48.357	1.00	27.55	B
ATOM	3204	CG2	VAL	93	23.807	5.170	49.178	1.00	29.02	B
ATOM	3205	C	VAL	93	20.771	5.339	46.843	1.00	24.60	B
ATOM	3206	O	VAL	93	19.759	5.955	47.110	1.00	24.17	B
ATOM	3207	N	ILE	94	21.175	5.150	45.596	1.00	22.93	B
ATOM	3208	CA	ILE	94	20.398	5.657	44.466	1.00	23.06	B
ATOM	3209	CB	ILE	94	21.193	5.441	43.130	1.00	22.09	B
ATOM	3210	CG2	ILE	94	20.367	5.867	41.905	1.00	18.23	B
ATOM	3211	CG1	ILE	94	22.498	6.262	43.205	1.00	20.00	B
ATOM	3212	CD1	ILE	94	23.382	6.115	42.021	1.00	18.08	B
ATOM	3213	C	ILE	94	18.984	5.036	44.384	1.00	23.71	B
ATOM	3214	O	ILE	94	18.079	5.630	43.845	1.00	24.46	B
ATOM	3215	N	MET	95	18.787	3.839	44.924	1.00	25.14	B
ATOM	3216	CA	MET	95	17.451	3.234	44.893	1.00	25.03	B
ATOM	3217	CB	MET	95	17.511	1.735	45.167	1.00	24.81	B
ATOM	3218	CG	MET	95	17.896	0.898	43.984	1.00	24.81	B
ATOM	3219	SD	MET	95	17.840	-0.821	44.434	1.00	28.44	B
ATOM	3220	CE	MET	95	19.568	-1.182	44.778	1.00	27.32	B
ATOM	3221	C	MET	95	16.585	3.864	45.977	1.00	25.84	B
ATOM	3222	O	MET	95	15.407	3.606	46.068	1.00	26.55	B
ATOM	3223	N	GLY	96	17.193	4.694	46.811	1.00	26.29	B
ATOM	3224	CA	GLY	96	16.417	5.335	47.854	1.00	26.67	B
ATOM	3225	C	GLY	96	16.650	4.824	49.264	1.00	28.04	B
ATOM	3226	O	GLY	96	15.864	5.121	50.170	1.00	29.08	B
ATOM	3227	N	TYR	97	17.733	4.075	49.454	1.00	28.81	B
ATOM	3228	CA	TYR	97	18.081	3.524	50.760	1.00	29.52	B
ATOM	3229	CB	TYR	97	18.680	2.117	50.591	1.00	31.73	B
ATOM	3230	CG	TYR	97	17.674	1.041	50.230	1.00	34.37	B
ATOM	3231	CD1	TYR	97	17.016	0.310	51.223	1.00	35.37	B
ATOM	3232	CE1	TYR	97	16.087	-0.663	50.904	1.00	36.70	B
ATOM	3233	CD2	TYR	97	17.370	0.769	48.901	1.00	35.61	B
ATOM	3234	CE2	TYR	97	16.439	-0.198	48.569	1.00	37.43	B
ATOM	3235	CZ	TYR	97	15.800	-0.909	49.575	1.00	38.91	B
ATOM	3236	OH	TYR	97	14.858	-1.862	49.257	1.00	40.43	B
ATOM	3237	C	TYR	97	19.090	4.391	51.528	1.00	28.25	B
ATOM	3238	O	TYR	97	19.819	5.172	50.943	1.00	29.03	B
ATOM	3239	N	ASN	98	19.107	4.266	52.850	1.00	26.29	B
ATOM	3240	CA	ASN	98	20.087	4.993	53.646	1.00	24.16	B
ATOM	3241	CB	ASN	98	19.520	5.396	54.994	1.00	23.70	B
ATOM	3242	CG	ASN	98	18.552	6.526	54.883	1.00	21.81	B
ATOM	3243	OD1	ASN	98	18.764	7.475	54.138	1.00	20.22	B
ATOM	3244	ND2	ASN	98	17.483	6.442	55.642	1.00	22.90	B
ATOM	3245	C	ASN	98	21.262	4.051	53.883	1.00	22.53	B
ATOM	3246	O	ASN	98	21.076	2.860	54.149	1.00	23.91	B
ATOM	3247	N	CYS	99	22.475	4.573	53.770	1.00	20.08	B
ATOM	3248	CA	CYS	99	23.652	3.741	53.976	1.00	16.35	B
ATOM	3249	CB	CYS	99	24.239	3.318	52.641	1.00	16.30	B
ATOM	3250	SG	CYS	99	23.128	2.271	51.748	1.00	16.76	B
ATOM	3251	C	CYS	99	24.717	4.437	54.786	1.00	13.97	B
ATOM	3252	O	CYS	99	24.764	5.664	54.867	1.00	13.48	B
ATOM	3253	N	THR	100	25.584	3.631	55.374	1.00	12.82	B
ATOM	3254	CA	THR	100	26.646	4.149	56.209	1.00	10.88	B
ATOM	3255	CB	THR	100	26.177	4.209	57.660	1.00	9.58	B

ATOM	3256	OG1	THR	100	25.155	5.204	57.768	1.00	6.29	B
ATOM	3257	CG2	THR	100	27.327	4.524	58.590	1.00	10.26	B
ATOM	3258	C	THR	100	27.874	3.264	56.104	1.00	10.53	B
ATOM	3259	O	THR	100	27.764	2.056	56.040	1.00	10.24	B
ATOM	3260	N	ILE	101	29.044	3.890	56.059	1.00	10.89	B
ATOM	3261	CA	ILE	101	30.303	3.156	55.993	1.00	12.11	B
ATOM	3262	CB	ILE	101	31.004	3.297	54.642	1.00	13.63	B
ATOM	3263	CG2	ILE	101	32.258	2.424	54.623	1.00	13.65	B
ATOM	3264	CG1	ILE	101	30.057	2.935	53.504	1.00	15.35	B
ATOM	3265	CD1	ILE	101	30.607	3.332	52.135	1.00	15.19	B
ATOM	3266	C	ILE	101	31.226	3.776	57.027	1.00	11.10	B
ATOM	3267	O	ILE	101	31.518	4.944	56.962	1.00	13.95	B
ATOM	3268	N	PHE	102	31.690	2.961	57.960	1.00	8.97	B
ATOM	3269	CA	PHE	102	32.569	3.412	59.024	1.00	5.36	B
ATOM	3270	CB	PHE	102	32.254	2.693	60.337	1.00	5.27	B
ATOM	3271	CG	PHE	102	30.964	3.097	60.979	1.00	3.08	B
ATOM	3272	CD1	PHE	102	30.912	4.233	61.785	1.00	3.17	B
ATOM	3273	CD2	PHE	102	29.821	2.315	60.839	1.00	1.92	B
ATOM	3274	CE1	PHE	102	29.737	4.591	62.458	1.00	2.33	B
ATOM	3275	CE2	PHE	102	28.648	2.667	61.505	1.00	1.69	B
ATOM	3276	CZ	PHE	102	28.608	3.812	62.323	1.00	1.17	B
ATOM	3277	C	PHE	102	33.974	2.937	58.708	1.00	4.97	B
ATOM	3278	O	PHE	102	34.160	1.984	57.997	1.00	6.23	B
ATOM	3279	N	ALA	103	34.956	3.641	59.244	1.00	5.31	B
ATOM	3280	CA	ALA	103	36.345	3.256	59.091	1.00	3.70	B
ATOM	3281	CB	ALA	103	37.115	4.337	58.408	1.00	2.97	B
ATOM	3282	C	ALA	103	36.781	3.126	60.546	1.00	3.79	B
ATOM	3283	O	ALA	103	36.811	4.105	61.266	1.00	4.80	B
ATOM	3284	N	TYR	104	37.086	1.908	60.981	1.00	3.80	B
ATOM	3285	CA	TYR	104	37.503	1.670	62.366	1.00	3.56	B
ATOM	3286	CB	TYR	104	36.507	0.751	63.061	1.00	2.47	B
ATOM	3287	CG	TYR	104	36.842	0.498	64.507	1.00	1.59	B
ATOM	3288	CD1	TYR	104	37.780	-0.465	64.875	1.00	1.99	B
ATOM	3289	CE1	TYR	104	38.079	-0.706	66.227	1.00	1.00	B
ATOM	3290	CD2	TYR	104	36.211	1.215	65.510	1.00	3.23	B
ATOM	3291	CE2	TYR	104	36.492	0.988	66.863	1.00	1.00	B
ATOM	3292	CZ	TYR	104	37.419	0.031	67.217	1.00	1.00	B
ATOM	3293	OH	TYR	104	37.667	-0.164	68.555	1.00	1.00	B
ATOM	3294	C	TYR	104	38.893	1.046	62.517	1.00	3.38	B
ATOM	3295	O	TYR	104	39.225	0.087	61.843	1.00	3.35	B
ATOM	3296	N	GLY	105	39.680	1.586	63.440	1.00	4.31	B
ATOM	3297	CA	GLY	105	41.024	1.088	63.646	1.00	5.04	B
ATOM	3298	C	GLY	105	41.931	2.086	64.335	1.00	5.61	B
ATOM	3299	O	GLY	105	41.560	3.226	64.565	1.00	5.55	B
ATOM	3300	N	GLN	106	43.132	1.627	64.657	1.00	7.21	B
ATOM	3301	CA	GLN	106	44.154	2.414	65.338	1.00	9.77	B
ATOM	3302	CB	GLN	106	45.303	1.473	65.701	1.00	11.84	B
ATOM	3303	CG	GLN	106	46.625	2.127	65.977	1.00	18.02	B
ATOM	3304	CD	GLN	106	47.651	1.110	66.407	1.00	20.93	B
ATOM	3305	OE1	GLN	106	47.887	0.126	65.707	1.00	20.58	B
ATOM	3306	NE2	GLN	106	48.265	1.333	67.569	1.00	24.16	B
ATOM	3307	C	GLN	106	44.684	3.603	64.525	1.00	9.05	B
ATOM	3308	O	GLN	106	44.759	3.535	63.318	1.00	8.64	B
ATOM	3309	N	THR	107	45.040	4.693	65.206	1.00	9.25	B
ATOM	3310	CA	THR	107	45.589	5.863	64.537	1.00	9.91	B
ATOM	3311	CB	THR	107	46.090	6.935	65.545	1.00	11.30	B
ATOM	3312	OG1	THR	107	44.998	7.433	66.328	1.00	12.57	B
ATOM	3313	CG2	THR	107	46.715	8.089	64.807	1.00	11.37	B
ATOM	3314	C	THR	107	46.784	5.384	63.720	1.00	9.43	B
ATOM	3315	O	THR	107	47.631	4.615	64.226	1.00	6.62	B
ATOM	3316	N	GLY	108	46.836	5.797	62.455	1.00	7.40	B
ATOM	3317	CA	GLY	108	47.956	5.419	61.613	1.00	7.87	B
ATOM	3318	C	GLY	108	47.801	4.136	60.815	1.00	7.55	B
ATOM	3319	O	GLY	108	48.771	3.609	60.263	1.00	10.21	B
ATOM	3320	N	THR	109	46.581	3.624	60.748	1.00	5.82	B
ATOM	3321	CA	THR	109	46.349	2.400	59.992	1.00	4.83	B
ATOM	3322	CB	THR	109	45.588	1.329	60.827	1.00	3.30	B
ATOM	3323	OG1	THR	109	44.316	1.824	61.248	1.00	2.94	B
ATOM	3324	CG2	THR	109	46.388	0.954	62.027	1.00	4.86	B
ATOM	3325	C	THR	109	45.611	2.616	58.675	1.00	5.10	B
ATOM	3326	O	THR	109	45.305	1.648	57.954	1.00	5.03	B
ATOM	3327	N	GLY	110	45.298	3.871	58.364	1.00	3.29	B
ATOM	3328	CA	GLY	110	44.613	4.141	57.122	1.00	1.90	B

ATOM	3329	C	GLY	110	43.131	4.484	57.097	1.00	2.61	B
ATOM	3330	O	GLY	110	42.521	4.385	56.025	1.00	1.00	B
ATOM	3331	N	LYS	111	42.539	4.885	58.227	1.00	4.13	B
ATOM	3332	CA	LYS	111	41.117	5.282	58.231	1.00	2.65	B
ATOM	3333	CB	LYS	111	40.636	5.636	59.651	1.00	2.73	B
ATOM	3334	CG	LYS	111	40.588	4.463	60.630	1.00	4.22	B
ATOM	3335	CD	LYS	111	39.990	4.860	61.974	1.00	1.25	B
ATOM	3336	CE	LYS	111	40.770	5.978	62.652	1.00	1.64	B
ATOM	3337	NZ	LYS	111	42.112	5.563	63.122	1.00	3.15	B
ATOM	3338	C	LYS	111	40.876	6.516	57.319	1.00	3.52	B
ATOM	3339	O	LYS	111	39.940	6.553	56.504	1.00	3.17	B
ATOM	3340	N	THR	112	41.738	7.515	57.421	1.00	2.71	B
ATOM	3341	CA	THR	112	41.536	8.697	56.607	1.00	4.38	B
ATOM	3342	CB	THR	112	42.245	9.927	57.209	1.00	3.24	B
ATOM	3343	OG1	THR	112	41.689	10.219	58.500	1.00	2.46	B
ATOM	3344	CG2	THR	112	42.049	11.122	56.306	1.00	5.02	B
ATOM	3345	C	THR	112	42.010	8.459	55.175	1.00	6.62	B
ATOM	3346	O	THR	112	41.499	9.074	54.223	1.00	5.92	B
ATOM	3347	N	PHE	113	42.974	7.556	55.013	1.00	7.30	B
ATOM	3348	CA	PHE	113	43.484	7.275	53.680	1.00	9.51	B
ATOM	3349	CB	PHE	113	44.690	6.342	53.705	1.00	11.02	B
ATOM	3350	CG	PHE	113	45.299	6.119	52.344	1.00	13.48	B
ATOM	3351	CD1	PHE	113	46.106	7.088	51.763	1.00	13.42	B
ATOM	3352	CD2	PHE	113	45.021	4.974	51.624	1.00	13.65	B
ATOM	3353	CE1	PHE	113	46.626	6.927	50.496	1.00	13.19	B
ATOM	3354	CE2	PHE	113	45.542	4.806	50.345	1.00	14.93	B
ATOM	3355	CZ	PHE	113	46.346	5.792	49.784	1.00	13.30	B
ATOM	3356	C	PHE	113	42.393	6.604	52.866	1.00	10.02	B
ATOM	3357	O	PHE	113	42.195	6.916	51.689	1.00	9.19	B
ATOM	3358	N	THR	114	41.686	5.686	53.519	1.00	9.92	B
ATOM	3359	CA	THR	114	40.601	4.946	52.905	1.00	8.86	B
ATOM	3360	CB	THR	114	40.157	3.792	53.812	1.00	9.97	B
ATOM	3361	OG1	THR	114	41.256	2.900	54.000	1.00	10.04	B
ATOM	3362	CG2	THR	114	39.026	3.006	53.174	1.00	10.07	B
ATOM	3363	C	THR	114	39.397	5.824	52.608	1.00	8.06	B
ATOM	3364	O	THR	114	38.935	5.875	51.496	1.00	8.14	B
ATOM	3365	N	MET	115	38.908	6.538	53.612	1.00	6.57	B
ATOM	3366	CA	MET	115	37.730	7.365	53.422	1.00	6.18	B
ATOM	3367	CB	MET	115	37.149	7.844	54.760	1.00	8.16	B
ATOM	3368	CG	MET	115	36.761	6.723	55.717	1.00	12.31	B
ATOM	3369	SD	MET	115	35.709	5.494	54.920	1.00	17.76	B
ATOM	3370	CE	MET	115	34.142	6.334	54.973	1.00	16.39	B
ATOM	3371	C	MET	115	37.903	8.594	52.570	1.00	6.31	B
ATOM	3372	O	MET	115	36.998	8.943	51.837	1.00	10.20	B
ATOM	3373	N	GLU	116	39.061	9.244	52.660	1.00	6.06	B
ATOM	3374	CA	GLU	116	39.295	10.476	51.909	1.00	2.45	B
ATOM	3375	CB	GLU	116	39.743	11.607	52.838	1.00	2.23	B
ATOM	3376	CG	GLU	116	38.737	11.962	53.924	1.00	1.00	B
ATOM	3377	CD	GLU	116	39.091	13.216	54.722	1.00	1.00	B
ATOM	3378	OE1	GLU	116	40.124	13.850	54.464	1.00	1.56	B
ATOM	3379	OE2	GLU	116	38.323	13.586	55.626	1.00	1.00	B
ATOM	3380	C	GLU	116	40.342	10.311	50.843	1.00	2.04	B
ATOM	3381	O	GLU	116	40.070	10.587	49.695	1.00	1.54	B
ATOM	3382	N	GLY	117	41.539	9.869	51.235	1.00	2.71	B
ATOM	3383	CA	GLY	117	42.603	9.663	50.263	1.00	3.19	B
ATOM	3384	C	GLY	117	43.531	10.842	50.294	1.00	1.91	B
ATOM	3385	O	GLY	117	43.293	11.739	51.033	1.00	2.28	B
ATOM	3386	N	GLU	118	44.568	10.822	49.466	1.00	3.14	B
ATOM	3387	CA	GLU	118	45.562	11.897	49.412	1.00	3.61	B
ATOM	3388	CB	GLU	118	46.879	11.427	50.051	1.00	3.14	B
ATOM	3389	CG	GLU	118	46.652	10.690	51.389	1.00	7.09	B
ATOM	3390	CD	GLU	118	47.933	10.200	52.062	1.00	9.57	B
ATOM	3391	OE1	GLU	118	48.831	9.748	51.317	1.00	11.82	B
ATOM	3392	OE2	GLU	118	48.030	10.259	53.317	1.00	6.51	B
ATOM	3393	C	GLU	118	45.813	12.253	47.959	1.00	4.59	B
ATOM	3394	O	GLU	118	45.209	11.670	47.063	1.00	4.23	B
ATOM	3395	N	ARG	119	46.681	13.221	47.713	1.00	7.04	B
ATOM	3396	CA	ARG	119	46.976	13.564	46.329	1.00	10.62	B
ATOM	3397	CB	ARG	119	47.171	15.067	46.131	1.00	10.38	B
ATOM	3398	CG	ARG	119	45.961	15.941	46.462	1.00	13.02	B
ATOM	3399	CD	ARG	119	44.705	15.414	45.837	1.00	13.25	B
ATOM	3400	NE	ARG	119	44.838	15.093	44.420	1.00	13.98	B
ATOM	3401	CZ	ARG	119	44.759	15.955	43.411	1.00	11.43	B

ATOM	3402	NH1	ARG	119	44.543	17.247	43.614	1.00	9.13	B
ATOM	3403	NH2	ARG	119	44.890	15.498	42.175	1.00	10.86	B
ATOM	3404	C	ARG	119	48.274	12.907	45.912	1.00	12.67	B
ATOM	3405	O	ARG	119	49.210	12.823	46.712	1.00	12.43	B
ATOM	3406	N	SER	120	48.328	12.416	44.675	1.00	15.44	B
ATOM	3407	CA	SER	120	49.563	11.812	44.182	1.00	17.48	B
ATOM	3408	CB	SER	120	49.392	11.272	42.755	1.00	18.24	B
ATOM	3409	OG	SER	120	48.605	10.090	42.735	1.00	19.78	B
ATOM	3410	C	SER	120	50.519	12.978	44.185	1.00	18.56	B
ATOM	3411	O	SER	120	50.161	14.050	43.772	1.00	20.75	B
ATOM	3412	N	PRO	121	51.748	12.782	44.660	1.00	20.06	B
ATOM	3413	CD	PRO	121	52.403	11.508	45.013	1.00	20.52	B
ATOM	3414	CA	PRO	121	52.700	13.896	44.686	1.00	20.89	B
ATOM	3415	CB	PRO	121	53.912	13.275	45.385	1.00	21.27	B
ATOM	3416	CG	PRO	121	53.881	11.834	44.872	1.00	21.35	B
ATOM	3417	C	PRO	121	53.028	14.538	43.332	1.00	21.75	B
ATOM	3418	O	PRO	121	52.835	13.918	42.270	1.00	21.17	B
ATOM	3419	N	ASN	122	53.514	15.785	43.393	1.00	21.50	B
ATOM	3420	CA	ASN	122	53.957	16.561	42.227	1.00	22.52	B
ATOM	3421	CB	ASN	122	55.199	15.865	41.632	1.00	24.29	B
ATOM	3422	CG	ASN	122	56.137	16.828	40.956	1.00	26.30	B
ATOM	3423	OD1	ASN	122	56.538	17.815	41.553	1.00	28.88	B
ATOM	3424	ND2	ASN	122	56.488	16.552	39.705	1.00	26.63	B
ATOM	3425	C	ASN	122	52.917	16.852	41.126	1.00	22.37	B
ATOM	3426	O	ASN	122	53.271	16.962	39.930	1.00	20.20	B
ATOM	3427	N	GLU	123	51.651	16.999	41.518	1.00	22.38	B
ATOM	3428	CA	GLU	123	50.573	17.294	40.561	1.00	22.86	B
ATOM	3429	CB	GLU	123	50.664	18.735	40.072	1.00	21.58	B
ATOM	3430	CG	GLU	123	50.338	19.754	41.110	1.00	21.60	B
ATOM	3431	CD	GLU	123	50.218	21.112	40.506	1.00	23.71	B
ATOM	3432	OE1	GLU	123	51.124	21.512	39.736	1.00	24.05	B
ATOM	3433	OE2	GLU	123	49.220	21.789	40.808	1.00	24.70	B
ATOM	3434	C	GLU	123	50.573	16.401	39.319	1.00	23.43	B
ATOM	3435	O	GLU	123	50.357	16.856	38.189	1.00	22.15	B
ATOM	3436	N	GLU	124	50.809	15.116	39.538	1.00	25.66	B
ATOM	3437	CA	GLU	124	50.840	14.186	38.435	1.00	27.17	B
ATOM	3438	CB	GLU	124	51.320	12.816	38.905	1.00	28.99	B
ATOM	3439	CG	GLU	124	51.698	11.884	37.763	1.00	33.91	B
ATOM	3440	CD	GLU	124	52.179	10.531	38.247	1.00	36.81	B
ATOM	3441	OE1	GLU	124	52.681	10.475	39.395	1.00	37.60	B
ATOM	3442	OE2	GLU	124	52.061	9.543	37.476	1.00	36.71	B
ATOM	3443	C	GLU	124	49.466	14.045	37.791	1.00	26.54	B
ATOM	3444	O	GLU	124	49.351	13.966	36.571	1.00	28.04	B
ATOM	3445	N	TYR	125	48.425	14.023	38.616	1.00	24.51	B
ATOM	3446	CA	TYR	125	47.065	13.864	38.117	1.00	22.37	B
ATOM	3447	CB	TYR	125	46.424	12.570	38.618	1.00	24.02	B
ATOM	3448	CG	TYR	125	47.232	11.305	38.445	1.00	24.34	B
ATOM	3449	CD1	TYR	125	48.215	10.951	39.372	1.00	24.16	B
ATOM	3450	CE1	TYR	125	48.938	9.770	39.238	1.00	24.97	B
ATOM	3451	CD2	TYR	125	46.994	10.440	37.368	1.00	23.29	B
ATOM	3452	CE2	TYR	125	47.715	9.257	37.224	1.00	23.28	B
ATOM	3453	CZ	TYR	125	48.685	8.927	38.165	1.00	25.16	B
ATOM	3454	OH	TYR	125	49.395	7.750	38.059	1.00	24.88	B
ATOM	3455	C	TYR	125	46.089	14.936	38.586	1.00	22.58	B
ATOM	3456	O	TYR	125	46.366	15.703	39.516	1.00	24.23	B
ATOM	3457	N	THR	126	44.941	14.984	37.920	1.00	21.47	B
ATOM	3458	CA	THR	126	43.889	15.919	38.280	1.00	20.00	B
ATOM	3459	CB	THR	126	42.913	16.147	37.140	1.00	20.72	B
ATOM	3460	OG1	THR	126	42.379	14.888	36.723	1.00	21.10	B
ATOM	3461	CG2	THR	126	43.598	16.837	35.984	1.00	20.85	B
ATOM	3462	C	THR	126	43.158	15.142	39.353	1.00	17.64	B
ATOM	3463	O	THR	126	43.223	13.940	39.359	1.00	16.55	B
ATOM	3464	N	TRP	127	42.441	15.820	40.241	1.00	16.83	B
ATOM	3465	CA	TRP	127	41.749	15.118	41.332	1.00	15.87	B
ATOM	3466	CB	TRP	127	40.927	16.080	42.213	1.00	14.78	B
ATOM	3467	CG	TRP	127	39.645	16.561	41.596	1.00	12.27	B
ATOM	3468	CD2	TRP	127	38.379	15.935	41.708	1.00	9.16	B
ATOM	3469	CE2	TRP	127	37.467	16.702	40.951	1.00	9.12	B
ATOM	3470	CE3	TRP	127	37.925	14.802	42.375	1.00	7.09	B
ATOM	3471	CD1	TRP	127	39.462	17.662	40.795	1.00	11.95	B
ATOM	3472	NE1	TRP	127	38.150	17.749	40.405	1.00	11.09	B
ATOM	3473	CZ2	TRP	127	36.142	16.366	40.845	1.00	8.67	B
ATOM	3474	CZ3	TRP	127	36.606	14.472	42.271	1.00	7.96	B

ATOM	3475	CH2	TRP	127	35.724	15.251	41.511	1.00	9.12	B
ATOM	3476	C	TRP	127	40.824	13.969	40.917	1.00	15.77	B
ATOM	3477	O	TRP	127	40.807	12.907	41.536	1.00	16.78	B
ATOM	3478	N	GLU	128	40.065	14.145	39.855	1.00	16.83	B
ATOM	3479	CA	GLU	128	39.168	13.073	39.465	1.00	16.42	B
ATOM	3480	CB	GLU	128	38.092	13.631	38.537	1.00	15.75	B
ATOM	3481	CG	GLU	128	38.578	14.230	37.234	1.00	14.47	B
ATOM	3482	CD	GLU	128	37.432	14.890	36.478	1.00	17.33	B
ATOM	3483	OE1	GLU	128	36.986	15.975	36.897	1.00	18.91	B
ATOM	3484	OE2	GLU	128	36.954	14.324	35.477	1.00	17.86	B
ATOM	3485	C	GLU	128	39.828	11.828	38.847	1.00	17.44	B
ATOM	3486	O	GLU	128	39.142	10.851	38.564	1.00	17.96	B
ATOM	3487	N	GLU	129	41.147	11.846	38.653	1.00	18.02	B
ATOM	3488	CA	GLU	129	41.836	10.692	38.078	1.00	19.12	B
ATOM	3489	CB	GLU	129	42.509	11.020	36.740	1.00	20.74	B
ATOM	3490	CG	GLU	129	41.574	11.402	35.595	1.00	26.16	B
ATOM	3491	CD	GLU	129	42.324	11.739	34.299	1.00	30.95	B
ATOM	3492	OE1	GLU	129	41.711	12.357	33.393	1.00	32.49	B
ATOM	3493	OE2	GLU	129	43.521	11.385	34.178	1.00	32.69	B
ATOM	3494	C	GLU	129	42.945	10.219	38.990	1.00	18.40	B
ATOM	3495	O	GLU	129	43.677	9.331	38.637	1.00	18.01	B
ATOM	3496	N	ASP	130	43.051	10.816	40.173	1.00	17.65	B
ATOM	3497	CA	ASP	130	44.115	10.465	41.113	1.00	17.80	B
ATOM	3498	CB	ASP	130	44.200	11.536	42.211	1.00	17.64	B
ATOM	3499	CG	ASP	130	45.540	11.556	42.908	1.00	19.83	B
ATOM	3500	OD1	ASP	130	46.026	10.466	43.291	1.00	20.74	B
ATOM	3501	OD2	ASP	130	46.097	12.661	43.070	1.00	20.64	B
ATOM	3502	C	ASP	130	43.843	9.091	41.704	1.00	17.66	B
ATOM	3503	O	ASP	130	42.792	8.867	42.302	1.00	18.25	B
ATOM	3504	N	PRO	131	44.778	8.141	41.521	1.00	17.22	B
ATOM	3505	CD	PRO	131	46.046	8.282	40.780	1.00	17.06	B
ATOM	3506	CA	PRO	131	44.617	6.778	42.052	1.00	16.05	B
ATOM	3507	CB	PRO	131	45.716	5.994	41.316	1.00	14.70	B
ATOM	3508	CG	PRO	131	46.802	7.019	41.154	1.00	17.48	B
ATOM	3509	C	PRO	131	44.668	6.713	43.589	1.00	15.30	B
ATOM	3510	O	PRO	131	44.318	5.697	44.187	1.00	14.37	B
ATOM	3511	N	LEU	132	45.114	7.797	44.226	1.00	15.18	B
ATOM	3512	CA	LEU	132	45.169	7.841	45.683	1.00	13.57	B
ATOM	3513	CB	LEU	132	46.380	8.644	46.165	1.00	12.21	B
ATOM	3514	CG	LEU	132	47.741	8.012	45.842	1.00	12.83	B
ATOM	3515	CD1	LEU	132	48.850	8.803	46.511	1.00	7.88	B
ATOM	3516	CD2	LEU	132	47.773	6.553	46.317	1.00	13.99	B
ATOM	3517	C	LEU	132	43.882	8.393	46.295	1.00	14.28	B
ATOM	3518	O	LEU	132	43.737	8.410	47.526	1.00	13.98	B
ATOM	3519	N	ALA	133	42.947	8.832	45.443	1.00	13.83	B
ATOM	3520	CA	ALA	133	41.651	9.342	45.909	1.00	12.82	B
ATOM	3521	CB	ALA	133	40.796	9.805	44.733	1.00	12.54	B
ATOM	3522	C	ALA	133	40.875	8.291	46.717	1.00	13.00	B
ATOM	3523	O	ALA	133	40.840	7.092	46.371	1.00	14.00	B
ATOM	3524	N	GLY	134	40.226	8.760	47.780	1.00	13.17	B
ATOM	3525	CA	GLY	134	39.470	7.884	48.653	1.00	10.45	B
ATOM	3526	C	GLY	134	37.996	7.819	48.324	1.00	9.48	B
ATOM	3527	O	GLY	134	37.546	8.422	47.385	1.00	8.50	B
ATOM	3528	N	ILE	135	37.254	7.094	49.158	1.00	10.67	B
ATOM	3529	CA	ILE	135	35.820	6.874	48.981	1.00	9.46	B
ATOM	3530	CB	ILE	135	35.237	6.087	50.180	1.00	9.70	B
ATOM	3531	CG2	ILE	135	33.709	5.990	50.079	1.00	10.21	B
ATOM	3532	CG1	ILE	135	35.837	4.686	50.214	1.00	8.19	B
ATOM	3533	CD1	ILE	135	35.426	3.864	51.452	1.00	8.61	B
ATOM	3534	C	ILE	135	34.968	8.115	48.739	1.00	9.92	B
ATOM	3535	O	ILE	135	34.135	8.150	47.812	1.00	7.51	B
ATOM	3536	N	ILE	136	35.157	9.136	49.560	1.00	9.63	B
ATOM	3537	CA	ILE	136	34.379	10.340	49.371	1.00	8.14	B
ATOM	3538	CB	ILE	136	34.671	11.371	50.500	1.00	6.28	B
ATOM	3539	CG2	ILE	136	33.997	12.691	50.166	1.00	6.74	B
ATOM	3540	CG1	ILE	136	34.125	10.825	51.831	1.00	5.22	B
ATOM	3541	CD1	ILE	136	34.553	11.574	53.070	1.00	1.00	B
ATOM	3542	C	ILE	136	34.538	10.992	47.978	1.00	9.33	B
ATOM	3543	O	ILE	136	33.569	11.242	47.274	1.00	10.23	B
ATOM	3544	N	PRO	137	35.767	11.252	47.552	1.00	7.86	B
ATOM	3545	CD	PRO	137	37.096	11.215	48.163	1.00	7.00	B
ATOM	3546	CA	PRO	137	35.816	11.874	46.234	1.00	7.00	B
ATOM	3547	CB	PRO	137	37.243	12.398	46.174	1.00	5.68	B

ATOM	3548	CG	PRO	137	37.968	11.448	46.976	1.00	7.36	B	
ATOM	3549	C	PRO	137	35.370	10.967	45.098	1.00	7.27	B	
ATOM	3550	O	PRO	137	34.857	11.434	44.120	1.00	9.92	B	
ATOM	3551	N	ARG	138	35.547	9.661	45.233	1.00	7.38	B	
ATOM	3552	CA	ARG	138	35.132	8.765	44.157	1.00	4.69	B	
ATOM	3553	CB	ARG	138	35.761	7.375	44.314	1.00	5.18	B	
ATOM	3554	CG	ARG	138	37.257	7.373	44.145	1.00	4.97	B	
ATOM	3555	CD	ARG	138	37.858	6.057	44.522	1.00	8.61	B	
ATOM	3556	NE	ARG	138	39.307	6.094	44.387	1.00	9.73	B	
ATOM	3557	CZ	ARG	138	39.954	5.973	43.235	1.00	12.02	B	
ATOM	3558	NH1	ARG	138	39.279	5.799	42.102	1.00	12.04	B	
ATOM	3559	NH2	ARG	138	41.280	6.028	43.216	1.00	13.69	B	
ATOM	3560	C	ARG	138	33.623	8.667	44.131	1.00	4.18	B	
ATOM	3561	O	ARG	138	33.017	8.611	43.094	1.00	7.46	B	
ATOM	3562	N	THR	139	33.013	8.666	45.295	1.00	3.72	B	
ATOM	3563	CA	THR	139	31.578	8.581	45.339	1.00	3.48	B	
ATOM	3564	CB	THR	139	31.103	8.436	46.792	1.00	2.17	B	
ATOM	3565	OG1	THR	139	31.647	7.220	47.321	1.00	4.08	B	
ATOM	3566	CG2	THR	139	29.586	8.366	46.872	1.00	1.00	B	
ATOM	3567	C	THR	139	30.956	9.798	44.677	1.00	4.20	B	
ATOM	3568	O	THR	139	30.178	9.666	43.727	1.00	5.38	B	
ATOM	3569	N	LEU	140	31.313	10.983	45.148	1.00	4.85	B	
ATOM	3570	CA	LEU	140	30.740	12.187	44.582	1.00	5.86	B	
ATOM	3571	CB	LEU	140	31.374	13.423	45.207	1.00	4.02	B	
ATOM	3572	CG	LEU	140	30.995	13.484	46.692	1.00	4.42	B	
ATOM	3573	CD1	LEU	140	31.695	14.631	47.363	1.00	6.86	B	
ATOM	3574	CD2	LEU	140	29.511	13.617	46.827	1.00	2.19	B	
ATOM	3575	C	LEU	140	30.902	12.211	43.091	1.00	8.32	B	
ATOM	3576	O	LEU	140	29.958	12.523	42.378	1.00	10.70	B	
ATOM	3577	N	HIS	141	32.085	11.853	42.611	1.00	9.41	B	
ATOM	3578	CA	HIS	141	32.315	11.876	41.180	1.00	11.42	B	
ATOM	3579	CB	HIS	141	33.753	11.465	40.836	1.00	12.95	B	
ATOM	3580	CG	HIS	141	34.064	11.523	39.364	1.00	15.31	B	
ATOM	3581	CD2	HIS	141	34.074	10.555	38.413	1.00	14.59	B	
ATOM	3582	ND1	HIS	141	34.404	12.693	38.713	1.00	17.05	B	
ATOM	3583	CE1	HIS	141	34.612	12.445	37.432	1.00	15.66	B	
ATOM	3584	NE2	HIS	141	34.418	11.154	37.225	1.00	15.55	B	
ATOM	3585	C	HIS	141	31.362	10.910	40.495	1.00	11.46	B	
ATOM	3586	O	HIS	141	30.727	11.239	39.499	1.00	12.67	B	
ATOM	3587	N	GLN	142	31.251	9.714	41.054	1.00	12.56	B	
ATOM	3588	CA	GLN	142	30.405	8.694	40.464	1.00	12.86	B	
ATOM	3589	CB	GLN	142	30.707	7.336	41.103	1.00	14.29	B	
ATOM	3590	CG	GLN	142	32.000	6.739	40.590	1.00	18.45	B	
ATOM	3591	CD	GLN	142	32.012	6.628	39.068	1.00	21.75	B	
ATOM	3592	OE1	GLN	142	31.349	5.751	38.489	1.00	23.11	B	
ATOM	3593	NE2	GLN	142	32.743	7.535	38.408	1.00	20.86	B	
ATOM	3594	C	GLN	142	28.915	8.984	40.473	1.00	12.11	B	
ATOM	3595	O	GLN	142	28.206	8.585	39.560	1.00	11.87	B	
ATOM	3596	N	ILE	143	28.434	9.664	41.506	1.00	11.12	B	
ATOM	3597	CA	ILE	143	27.018	10.010	41.573	1.00	12.39	B	
ATOM	3598	CB	ILE	143	26.722	10.953	42.788	1.00	12.55	B	
ATOM	3599	CG2	ILE	143	25.341	11.608	42.650	1.00	12.75	B	
ATOM	3600	CG1	ILE	143	26.784	10.147	44.093	1.00	13.10	B	
ATOM	3601	CD1	ILE	143	26.532	10.971	45.338	1.00	10.72	B	
ATOM	3602	C	ILE	143	26.587	10.710	40.275	1.00	13.82	B	
ATOM	3603	O	ILE	143	25.541	10.391	39.705	1.00	14.18	B	
ATOM	3604	N	PHE	144	27.397	11.666	39.816	1.00	14.48	B	
ATOM	3605	CA	PHE	144	27.099	12.430	38.605	1.00	15.02	B	
ATOM	3606	CB	PHE	144	28.023	13.646	38.513	1.00	14.03	B	
ATOM	3607	CG	PHE	144	27.773	14.676	39.585	1.00	12.67	B	
ATOM	3608	CD1	PHE	144	26.680	15.527	39.510	1.00	10.36	B	
ATOM	3609	CD2	PHE	144	28.623	14.796	40.678	1.00	13.84	B	
ATOM	3610	CE1	PHE	144	26.442	16.473	40.498	1.00	9.69	B	
ATOM	3611	CE2	PHE	144	28.375	15.761	41.680	1.00	13.70	B	
ATOM	3612	CZ	PHE	144	27.286	16.591	41.578	1.00	11.21	B	
ATOM	3613	C	PHE	144	27.223	11.586	37.348	1.00	16.57	B	
ATOM	3614	O	PHE	144	26.516	11.835	36.384	1.00	16.66	B	
ATOM	3615	N	GLU	145	28.123	10.593	37.364	1.00	20.10	B	
ATOM	3616	CA	GLU	145	28.335	9.691	36.210	1.00	22.03	B	
ATOM	3617	CB	GLU	145	29.597	8.825	36.352	1.00	26.12	B	
ATOM	3618	CG	GLU	145	30.902	9.538	36.044	1.00	32.68	B	
ATOM	3619	CD	GLU	145	31.004	9.949	34.595	1.00	36.87	B	
ATOM	3620	OE1	GLU	145	31.965	10.666	34.249	1.00	39.57	B	

ATOM	3621	OE2	GLU	145	30.121	9.549	33.807	1.00	40.00	B
ATOM	3622	C	GLU	145	27.194	8.705	36.029	1.00	21.04	B
ATOM	3623	O	GLU	145	26.750	8.470	34.943	1.00	20.94	B
ATOM	3624	N	LYS	146	26.728	8.129	37.127	1.00	22.01	B
ATOM	3625	CA	LYS	146	25.628	7.166	37.072	1.00	22.94	B
ATOM	3626	CB	LYS	146	25.489	6.433	38.423	1.00	24.69	B
ATOM	3627	CG	LYS	146	26.725	5.599	38.799	1.00	27.30	B
ATOM	3628	CD	LYS	146	26.480	4.519	39.854	1.00	24.53	B
ATOM	3629	CE	LYS	146	27.560	3.447	39.715	1.00	25.61	B
ATOM	3630	NZ	LYS	146	27.404	2.262	40.595	1.00	24.71	B
ATOM	3631	C	LYS	146	24.281	7.799	36.702	1.00	24.00	B
ATOM	3632	O	LYS	146	23.472	7.178	36.020	1.00	24.07	B
ATOM	3633	N	LEU	147	24.049	9.035	37.138	1.00	23.75	B
ATOM	3634	CA	LEU	147	22.788	9.720	36.850	1.00	24.08	B
ATOM	3635	CB	LEU	147	22.247	10.365	38.123	1.00	24.33	B
ATOM	3636	CG	LEU	147	21.976	9.460	39.325	1.00	24.88	B
ATOM	3637	CD1	LEU	147	21.607	10.299	40.537	1.00	24.59	B
ATOM	3638	CD2	LEU	147	20.847	8.493	39.014	1.00	24.04	B
ATOM	3639	C	LEU	147	22.895	10.796	35.762	1.00	25.02	B
ATOM	3640	O	LEU	147	22.110	11.755	35.736	1.00	22.56	B
ATOM	3641	N	THR	148	23.857	10.627	34.857	1.00	27.04	B
ATOM	3642	CA	THR	148	24.073	11.585	33.774	1.00	28.40	B
ATOM	3643	CB	THR	148	25.296	11.194	32.905	1.00	28.80	B
ATOM	3644	OG1	THR	148	25.479	12.150	31.850	1.00	29.27	B
ATOM	3645	CG2	THR	148	25.108	9.794	32.318	1.00	30.26	B
ATOM	3646	C	THR	148	22.855	11.738	32.865	1.00	28.70	B
ATOM	3647	O	THR	148	22.466	12.848	32.580	1.00	29.54	B
ATOM	3648	N	ASP	149	22.253	10.638	32.413	1.00	27.95	B
ATOM	3649	CA	ASP	149	21.087	10.749	31.533	1.00	28.50	B
ATOM	3650	CB	ASP	149	21.500	11.014	30.067	1.00	28.76	B
ATOM	3651	CG	ASP	149	22.520	10.010	29.522	1.00	29.99	B
ATOM	3652	OD1	ASP	149	22.501	8.830	29.939	1.00	29.75	B
ATOM	3653	OD2	ASP	149	23.332	10.408	28.646	1.00	29.41	B
ATOM	3654	C	ASP	149	20.148	9.551	31.576	1.00	28.84	B
ATOM	3655	O	ASP	149	19.636	9.096	30.555	1.00	27.84	B
ATOM	3656	N	ASN	150	19.899	9.055	32.778	1.00	29.57	B
ATOM	3657	CA	ASN	150	19.008	7.912	32.928	1.00	31.21	B
ATOM	3658	CB	ASN	150	19.483	7.010	34.080	1.00	29.55	B
ATOM	3659	CG	ASN	150	19.259	7.641	35.459	1.00	28.21	B
ATOM	3660	OD1	ASN	150	19.347	8.859	35.618	1.00	27.26	B
ATOM	3661	ND2	ASN	150	18.969	6.804	36.458	1.00	25.05	B
ATOM	3662	C	ASN	150	17.550	8.345	33.175	1.00	31.80	B
ATOM	3663	O	ASN	150	16.693	7.501	33.485	1.00	32.95	B
ATOM	3664	N	GLY	151	17.279	9.648	33.043	1.00	30.56	B
ATOM	3665	CA	GLY	151	15.939	10.169	33.247	1.00	29.70	B
ATOM	3666	C	GLY	151	15.601	10.387	34.701	1.00	29.38	B
ATOM	3667	O	GLY	151	14.462	10.518	35.052	1.00	29.95	B
ATOM	3668	N	THR	152	16.616	10.412	35.549	1.00	29.90	B
ATOM	3669	CA	THR	152	16.386	10.634	36.964	1.00	30.17	B
ATOM	3670	CB	THR	152	17.082	9.552	37.805	1.00	29.93	B
ATOM	3671	OG1	THR	152	16.662	8.249	37.373	1.00	29.92	B
ATOM	3672	CG2	THR	152	16.739	9.730	39.272	1.00	31.14	B
ATOM	3673	C	THR	152	16.902	12.022	37.384	1.00	31.11	B
ATOM	3674	O	THR	152	18.104	12.232	37.543	1.00	32.13	B
ATOM	3675	N	GLU	153	15.977	12.968	37.531	1.00	30.29	B
ATOM	3676	CA	GLU	153	16.310	14.325	37.948	1.00	28.58	B
ATOM	3677	CB	GLU	153	15.041	15.174	37.977	1.00	31.74	B
ATOM	3678	CG	GLU	153	15.257	16.669	37.853	1.00	35.57	B
ATOM	3679	CD	GLU	153	15.641	17.082	36.438	1.00	38.01	B
ATOM	3680	OE1	GLU	153	15.923	18.281	36.200	1.00	38.59	B
ATOM	3681	OE2	GLU	153	15.655	16.201	35.551	1.00	39.17	B
ATOM	3682	C	GLU	153	16.861	14.173	39.366	1.00	25.90	B
ATOM	3683	O	GLU	153	16.382	13.346	40.114	1.00	25.18	B
ATOM	3684	N	PHE	154	17.852	14.978	39.738	1.00	24.45	B
ATOM	3685	CA	PHE	154	18.447	14.852	41.074	1.00	21.39	B
ATOM	3686	CB	PHE	154	19.411	13.651	41.115	1.00	20.65	B
ATOM	3687	CG	PHE	154	20.679	13.846	40.306	1.00	20.31	B
ATOM	3688	CD1	PHE	154	21.853	14.284	40.904	1.00	19.86	B
ATOM	3689	CD2	PHE	154	20.698	13.570	38.945	1.00	19.64	B
ATOM	3690	CE1	PHE	154	23.021	14.435	40.142	1.00	21.56	B
ATOM	3691	CE2	PHE	154	21.856	13.720	38.194	1.00	20.70	B
ATOM	3692	CZ	PHE	154	23.017	14.149	38.786	1.00	19.85	B
ATOM	3693	C	PHE	154	19.224	16.073	41.567	1.00	19.03	B

ATOM	3694	O	PHE	154	19.579	16.970	40.805	1.00	18.07		B
ATOM	3695	N	SER	155	19.470	16.107	42.865	1.00	17.25		B
ATOM	3696	CA	SER	155	20.234	17.200	43.451	1.00	17.56		B
ATOM	3697	CB	SER	155	19.310	18.302	44.043	1.00	18.40		B
ATOM	3698	OG	SER	155	18.744	17.999	45.315	1.00	19.07		B
ATOM	3699	C	SER	155	21.072	16.536	44.521	1.00	16.97		B
ATOM	3700	O	SER	155	20.629	15.587	45.157	1.00	15.32		B
ATOM	3701	N	VAL	156	22.286	17.034	44.708	1.00	17.21		B
ATOM	3702	CA	VAL	156	23.181	16.479	45.709	1.00	15.73		B
ATOM	3703	CB	VAL	156	24.452	15.964	45.066	1.00	16.35		B
ATOM	3704	CG1	VAL	156	25.307	15.319	46.089	1.00	16.70		B
ATOM	3705	CG2	VAL	156	24.117	14.993	43.973	1.00	18.36		B
ATOM	3706	C	VAL	156	23.577	17.503	46.762	1.00	14.63		B
ATOM	3707	O	VAL	156	24.031	18.595	46.441	1.00	12.84		B
ATOM	3708	N	LYS	157	23.394	17.138	48.024	1.00	15.08		B
ATOM	3709	CA	LYS	157	23.739	18.019	49.139	1.00	16.33		B
ATOM	3710	CB	LYS	157	22.485	18.370	49.962	1.00	17.27		B
ATOM	3711	CG	LYS	157	21.640	19.492	49.381	1.00	19.38		B
ATOM	3712	CD	LYS	157	20.323	19.704	50.121	1.00	19.23		B
ATOM	3713	CE	LYS	157	19.563	20.911	49.535	1.00	20.48		B
ATOM	3714	NZ	LYS	157	20.216	22.239	49.815	1.00	19.89		B
ATOM	3715	C	LYS	157	24.738	17.288	50.025	1.00	15.63		B
ATOM	3716	O	LYS	157	24.568	16.118	50.305	1.00	17.71		B
ATOM	3717	N	VAL	158	25.789	17.979	50.447	1.00	14.09		B
ATOM	3718	CA	VAL	158	26.782	17.350	51.313	1.00	12.31		B
ATOM	3719	CB	VAL	158	28.184	17.314	50.670	1.00	11.69		B
ATOM	3720	CG1	VAL	158	28.150	16.490	49.405	1.00	12.25		B
ATOM	3721	CG2	VAL	158	28.657	18.731	50.367	1.00	11.55		B
ATOM	3722	C	VAL	158	26.911	18.070	52.636	1.00	11.94		B
ATOM	3723	O	VAL	158	26.668	19.270	52.726	1.00	11.97		B
ATOM	3724	N	SER	159	27.301	17.321	53.659	1.00	10.91		B
ATOM	3725	CA	SER	159	27.490	17.876	54.992	1.00	11.22		B
ATOM	3726	CB	SER	159	26.245	17.662	55.846	1.00	11.02		B
ATOM	3727	OG	SER	159	25.184	18.476	55.385	1.00	17.68		B
ATOM	3728	C	SER	159	28.677	17.212	55.667	1.00	11.18		B
ATOM	3729	O	SER	159	28.925	16.002	55.499	1.00	10.26		B
ATOM	3730	N	LEU	160	29.431	18.011	56.405	1.00	11.19		B
ATOM	3731	CA	LEU	160	30.583	17.495	57.115	1.00	11.64		B
ATOM	3732	CB	LEU	160	31.875	18.043	56.498	1.00	11.99		B
ATOM	3733	CG	LEU	160	33.168	17.440	57.061	1.00	12.29		B
ATOM	3734	CD1	LEU	160	33.088	15.915	57.170	1.00	12.16		B
ATOM	3735	CD2	LEU	160	34.307	17.848	56.170	1.00	13.02		B
ATOM	3736	C	LEU	160	30.476	17.836	58.606	1.00	12.31		B
ATOM	3737	O	LEU	160	30.894	18.913	59.056	1.00	13.72		B
ATOM	3738	N	LEU	161	29.921	16.899	59.365	1.00	11.68		B
ATOM	3739	CA	LEU	161	29.728	17.056	60.794	1.00	11.73		B
ATOM	3740	CB	LEU	161	28.387	16.462	61.184	1.00	10.86		B
ATOM	3741	CG	LEU	161	28.069	16.373	62.667	1.00	11.21		B
ATOM	3742	CD1	LEU	161	28.038	17.772	63.257	1.00	14.64		B
ATOM	3743	CD2	LEU	161	26.735	15.687	62.849	1.00	11.87		B
ATOM	3744	C	LEU	161	30.805	16.318	61.565	1.00	11.76		B
ATOM	3745	O	LEU	161	31.023	15.148	61.353	1.00	14.92		B
ATOM	3746	N	GLU	162	31.493	17.005	62.461	1.00	11.26		B
ATOM	3747	CA	GLU	162	32.536	16.335	63.230	1.00	10.12		B
ATOM	3748	CB	GLU	162	33.914	16.845	62.829	1.00	9.47		B
ATOM	3749	CG	GLU	162	34.143	16.845	61.353	1.00	9.35		B
ATOM	3750	CD	GLU	162	35.607	16.813	61.008	1.00	9.38		B
ATOM	3751	OE1	GLU	162	36.443	17.239	61.829	1.00	9.19		B
ATOM	3752	OE2	GLU	162	35.929	16.357	59.901	1.00	8.99		B
ATOM	3753	C	GLU	162	32.339	16.498	64.729	1.00	10.38		B
ATOM	3754	O	GLU	162	31.849	17.527	65.222	1.00	7.96		B
ATOM	3755	N	ILE	163	32.734	15.456	65.444	1.00	10.66		B
ATOM	3756	CA	ILE	163	32.581	15.414	66.879	1.00	10.98		B
ATOM	3757	CB	ILE	163	31.782	14.160	67.293	1.00	11.27		B
ATOM	3758	CG2	ILE	163	31.505	14.192	68.793	1.00	11.05		B
ATOM	3759	CG1	ILE	163	30.504	14.066	66.462	1.00	11.37		B
ATOM	3760	CD1	ILE	163	29.804	12.728	66.528	1.00	12.73		B
ATOM	3761	C	ILE	163	33.941	15.387	67.559	1.00	10.94		B
ATOM	3762	O	ILE	163	34.849	14.680	67.127	1.00	11.24		B
ATOM	3763	N	TYR	164	34.071	16.177	68.619	1.00	10.16		B
ATOM	3764	CA	TYR	164	35.303	16.245	69.376	1.00	8.14		B
ATOM	3765	CB	TYR	164	36.254	17.270	68.759	1.00	5.82		B
ATOM	3766	CG	TYR	164	37.517	17.425	69.533	1.00	3.86		B

ATOM	3767	CD1	TYR	164	37.560	18.215	70.682	1.00	5.62	B
ATOM	3768	CE1	TYR	164	38.709	18.292	71.465	1.00	4.56	B
ATOM	3769	CD2	TYR	164	38.651	16.719	69.177	1.00	3.71	B
ATOM	3770	CE2	TYR	164	39.811	16.786	69.955	1.00	5.19	B
ATOM	3771	CZ	TYR	164	39.827	17.577	71.094	1.00	4.77	B
ATOM	3772	OH	TYR	164	40.976	17.675	71.832	1.00	5.42	B
ATOM	3773	C	TYR	164	34.937	16.617	70.802	1.00	8.94	B
ATOM	3774	O	TYR	164	34.299	17.627	71.061	1.00	9.91	B
ATOM	3775	N	ASN	165	35.346	15.775	71.731	1.00	10.87	B
ATOM	3776	CA	ASN	165	35.050	16.003	73.134	1.00	12.54	B
ATOM	3777	CB	ASN	165	35.847	17.192	73.674	1.00	15.11	B
ATOM	3778	CG	ASN	165	35.722	17.336	75.190	1.00	19.28	B
ATOM	3779	OD1	ASN	165	35.971	16.385	75.936	1.00	21.80	B
ATOM	3780	ND2	ASN	165	35.345	18.528	75.651	1.00	20.20	B
ATOM	3781	C	ASN	165	33.562	16.262	73.308	1.00	12.20	B
ATOM	3782	O	ASN	165	33.160	17.158	74.000	1.00	10.80	B
ATOM	3783	N	GLU	166	32.767	15.430	72.646	1.00	16.33	B
ATOM	3784	CA	GLU	166	31.304	15.495	72.656	1.00	18.28	B
ATOM	3785	CB	GLU	166	30.739	15.101	74.031	1.00	17.10	B
ATOM	3786	CG	GLU	166	30.887	13.610	74.353	1.00	16.82	B
ATOM	3787	CD	GLU	166	30.175	12.693	73.357	1.00	16.06	B
ATOM	3788	OE1	GLU	166	28.928	12.606	73.360	1.00	13.96	B
ATOM	3789	OE2	GLU	166	30.880	12.055	72.559	1.00	15.35	B
ATOM	3790	C	GLU	166	30.697	16.825	72.201	1.00	19.60	B
ATOM	3791	O	GLU	166	29.604	17.192	72.606	1.00	19.36	B
ATOM	3792	N	GLU	167	31.427	17.546	71.357	1.00	21.89	B
ATOM	3793	CA	GLU	167	30.956	18.818	70.823	1.00	22.41	B
ATOM	3794	CB	GLU	167	31.910	19.947	71.208	1.00	24.57	B
ATOM	3795	CG	GLU	167	31.998	20.181	72.701	1.00	28.83	B
ATOM	3796	CD	GLU	167	32.847	21.376	73.044	1.00	31.70	B
ATOM	3797	OE1	GLU	167	33.985	21.472	72.521	1.00	32.58	B
ATOM	3798	OE2	GLU	167	32.373	22.214	73.840	1.00	33.47	B
ATOM	3799	C	GLU	167	30.874	18.683	69.314	1.00	21.24	B
ATOM	3800	O	GLU	167	31.689	17.997	68.700	1.00	20.64	B
ATOM	3801	N	LEU	168	29.879	19.328	68.717	1.00	20.17	B
ATOM	3802	CA	LEU	168	29.712	19.254	67.269	1.00	19.71	B
ATOM	3803	CB	LEU	168	28.240	19.110	66.887	1.00	19.82	B
ATOM	3804	CG	LEU	168	27.430	17.954	67.457	1.00	19.46	B
ATOM	3805	CD1	LEU	168	28.198	16.653	67.320	1.00	19.39	B
ATOM	3806	CD2	LEU	168	27.113	18.236	68.903	1.00	20.70	B
ATOM	3807	C	LEU	168	30.251	20.477	66.524	1.00	19.80	B
ATOM	3808	O	LEU	168	30.055	21.611	66.939	1.00	20.40	B
ATOM	3809	N	PHE	169	30.928	20.229	65.411	1.00	19.38	B
ATOM	3810	CA	PHE	169	31.478	21.306	64.612	1.00	17.82	B
ATOM	3811	CB	PHE	169	33.004	21.327	64.706	1.00	17.88	B
ATOM	3812	CG	PHE	169	33.513	21.530	66.097	1.00	16.09	B
ATOM	3813	CD1	PHE	169	33.737	20.445	66.928	1.00	15.76	B
ATOM	3814	CD2	PHE	169	33.695	22.810	66.600	1.00	16.92	B
ATOM	3815	CE1	PHE	169	34.130	20.621	68.235	1.00	16.10	B
ATOM	3816	CE2	PHE	169	34.090	23.001	67.907	1.00	17.09	B
ATOM	3817	CZ	PHE	169	34.308	21.901	68.731	1.00	16.73	B
ATOM	3818	C	PHE	169	31.068	21.102	63.166	1.00	18.77	B
ATOM	3819	O	PHE	169	30.929	19.980	62.704	1.00	18.62	B
ATOM	3820	N	ASP	170	30.871	22.206	62.459	1.00	20.24	B
ATOM	3821	CA	ASP	170	30.476	22.171	61.055	1.00	21.83	B
ATOM	3822	CB	ASP	170	29.387	23.216	60.785	1.00	20.71	B
ATOM	3823	CG	ASP	170	28.832	23.135	59.382	1.00	22.77	B
ATOM	3824	OD1	ASP	170	29.510	22.563	58.493	1.00	23.50	B
ATOM	3825	OD2	ASP	170	27.724	23.658	59.158	1.00	24.44	B
ATOM	3826	C	ASP	170	31.714	22.545	60.269	1.00	22.03	B
ATOM	3827	O	ASP	170	32.119	23.693	60.281	1.00	23.16	B
ATOM	3828	N	LEU	171	32.320	21.577	59.593	1.00	21.95	B
ATOM	3829	CA	LEU	171	33.514	21.878	58.828	1.00	22.12	B
ATOM	3830	CB	LEU	171	34.449	20.674	58.827	1.00	20.38	B
ATOM	3831	CG	LEU	171	35.422	20.605	60.013	1.00	21.16	B
ATOM	3832	CD1	LEU	171	36.359	21.824	60.018	1.00	20.44	B
ATOM	3833	CD2	LEU	171	34.645	20.544	61.307	1.00	18.78	B
ATOM	3834	C	LEU	171	33.271	22.356	57.402	1.00	24.20	B
ATOM	3835	O	LEU	171	34.201	22.357	56.582	1.00	24.74	B
ATOM	3836	N	LEU	172	32.034	22.764	57.108	1.00	26.40	B
ATOM	3837	CA	LEU	172	31.686	23.266	55.776	1.00	28.39	B
ATOM	3838	CB	LEU	172	30.802	22.283	55.004	1.00	28.49	B
ATOM	3839	CG	LEU	172	31.536	21.056	54.448	1.00	29.54	B

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ATOM   3840  CD1 LEU   172      30.562  20.216  53.633  1.00 30.71      B
ATOM   3841  CD2 LEU   172      32.730  21.477  53.583  1.00 28.53      B
ATOM   3842  C   LEU   172      30.979  24.607  55.797  1.00 28.89      B
ATOM   3843  O   LEU   172      30.416  25.030  54.823  1.00 30.09      B
ATOM   3844  N   ASN   173      31.007  25.264  56.941  1.00 31.10      B
ATOM   3845  CA  ASN   173      30.403  26.580  57.043  1.00 34.00      B
ATOM   3846  CB  ASN   173      29.606  26.708  58.347  1.00 33.23      B
ATOM   3847  CG  ASN   173      28.903  28.053  58.473  1.00 32.72      B
ATOM   3848  OD1 ASN   173      28.108  28.268  59.381  1.00 33.30      B
ATOM   3849  ND2 ASN   173      29.205  28.967  57.551  1.00 31.17      B
ATOM   3850  C   ASN   173      31.554  27.579  56.982  1.00 35.93      B
ATOM   3851  O   ASN   173      32.402  27.627  57.861  1.00 35.47      B
ATOM   3852  N   PRO   174      31.609  28.372  55.908  1.00 38.25      B
ATOM   3853  CD  PRO   174      30.799  28.283  54.681  1.00 38.57      B
ATOM   3854  CA  PRO   174      32.674  29.362  55.753  1.00 40.38      B
ATOM   3855  CB  PRO   174      32.702  29.569  54.242  1.00 39.65      B
ATOM   3856  CG  PRO   174      31.264  29.478  53.900  1.00 38.79      B
ATOM   3857  C   PRO   174      32.445  30.632  56.582  1.00 42.95      B
ATOM   3858  O   PRO   174      33.356  31.450  56.743  1.00 43.55      B
ATOM   3859  N   SER   175      31.234  30.794  57.108  1.00 45.10      B
ATOM   3860  CA  SER   175      30.906  31.974  57.913  1.00 47.15      B
ATOM   3861  CB  SER   175      29.395  32.227  57.889  1.00 47.30      B
ATOM   3862  OG  SER   175      28.906  32.331  56.559  1.00 49.37      B
ATOM   3863  C   SER   175      31.369  31.882  59.376  1.00 47.57      B
ATOM   3864  O   SER   175      31.800  32.872  59.970  1.00 48.25      B
ATOM   3865  N   SER   176      31.280  30.690  59.953  1.00 47.97      B
ATOM   3866  CA  SER   176      31.677  30.487  61.340  1.00 47.64      B
ATOM   3867  CB  SER   176      30.720  29.520  62.034  1.00 46.90      B
ATOM   3868  OG  SER   176      30.794  28.230  61.447  1.00 46.36      B
ATOM   3869  C   SER   176      33.083  29.917  61.451  1.00 48.54      B
ATOM   3870  O   SER   176      33.650  29.434  60.484  1.00 48.78      B
ATOM   3871  N   ASP   177      33.646  29.989  62.648  1.00 49.43      B
ATOM   3872  CA  ASP   177      34.979  29.467  62.874  1.00 50.07      B
ATOM   3873  CB  ASP   177      35.843  30.521  63.591  1.00 51.58      B
ATOM   3874  CG  ASP   177      35.342  30.852  64.996  1.00 53.37      B
ATOM   3875  OD1 ASP   177      35.948  31.723  65.658  1.00 54.70      B
ATOM   3876  OD2 ASP   177      34.353  30.246  65.452  1.00 54.61      B
ATOM   3877  C   ASP   177      34.880  28.160  63.669  1.00 49.81      B
ATOM   3878  O   ASP   177      33.833  27.830  64.235  1.00 48.89      B
ATOM   3879  N   VAL   178      35.980  27.422  63.707  1.00 49.42      B
ATOM   3880  CA  VAL   178      36.030  26.146  64.409  1.00 50.03      B
ATOM   3881  CB  VAL   178      37.385  25.452  64.150  1.00 50.76      B
ATOM   3882  CG1 VAL   178      37.528  25.131  62.665  1.00 49.77      B
ATOM   3883  CG2 VAL   178      38.538  26.353  64.629  1.00 50.93      B
ATOM   3884  C   VAL   178      35.791  26.203  65.927  1.00 49.82      B
ATOM   3885  O   VAL   178      35.912  25.194  66.623  1.00 50.17      B
ATOM   3886  N   SER   179      35.451  27.372  66.447  1.00 48.85      B
ATOM   3887  CA  SER   179      35.225  27.491  67.877  1.00 47.91      B
ATOM   3888  CB  SER   179      35.912  28.749  68.397  1.00 48.14      B
ATOM   3889  OG  SER   179      35.472  29.884  67.667  1.00 47.90      B
ATOM   3890  C   SER   179      33.739  27.541  68.211  1.00 47.46      B
ATOM   3891  O   SER   179      33.357  27.618  69.376  1.00 47.10      B
ATOM   3892  N   GLU   180      32.900  27.495  67.182  1.00 46.50      B
ATOM   3893  CA  GLU   180      31.458  27.542  67.383  1.00 45.18      B
ATOM   3894  CB  GLU   180      30.835  28.527  66.383  1.00 44.47      B
ATOM   3895  CG  GLU   180      31.026  29.983  66.788  1.00 44.05      B
ATOM   3896  CD  GLU   180      30.595  30.971  65.724  1.00 43.63      B
ATOM   3897  OE1 GLU   180      31.354  31.176  64.751  1.00 43.67      B
ATOM   3898  OE2 GLU   180      29.495  31.542  65.860  1.00 42.55      B
ATOM   3899  C   GLU   180      30.813  26.156  67.295  1.00 44.60      B
ATOM   3900  O   GLU   180      30.714  25.570  66.228  1.00 44.37      B
ATOM   3901  N   ARG   181      30.373  25.650  68.445  1.00 44.01      B
ATOM   3902  CA  ARG   181      29.739  24.342  68.529  1.00 42.83      B
ATOM   3903  CB  ARG   181      29.775  23.806  69.958  1.00 45.18      B
ATOM   3904  CG  ARG   181      28.755  24.439  70.895  1.00 47.37      B
ATOM   3905  CD  ARG   181      28.693  23.644  72.187  1.00 51.45      B
ATOM   3906  NE  ARG   181      27.541  23.972  73.034  1.00 54.79      B
ATOM   3907  CZ  ARG   181      26.267  23.753  72.706  1.00 56.32      B
ATOM   3908  NH1 ARG   181      25.969  23.205  71.539  1.00 57.53      B
ATOM   3909  NH2 ARG   181      25.286  24.065  73.548  1.00 56.18      B
ATOM   3910  C   ARG   181      28.278  24.404  68.121  1.00 40.59      B
ATOM   3911  O   ARG   181      27.632  25.414  68.254  1.00 41.20      B
ATOM   3912  N   LEU   182      27.759  23.293  67.632  1.00 38.61      B
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ATOM	3913	CA	LEU	182	26.370	23.253	67.219	1.00	35.94	B
ATOM	3914	CB	LEU	182	26.259	22.490	65.897	1.00	34.47	B
ATOM	3915	CG	LEU	182	27.018	23.098	64.718	1.00	31.55	B
ATOM	3916	CD1	LEU	182	26.951	22.179	63.525	1.00	30.32	B
ATOM	3917	CD2	LEU	182	26.417	24.440	64.382	1.00	29.89	B
ATOM	3918	C	LEU	182	25.532	22.579	68.300	1.00	35.46	B
ATOM	3919	O	LEU	182	26.057	21.845	69.139	1.00	35.35	B
ATOM	3920	N	GLN	183	24.227	22.839	68.270	1.00	35.14	B
ATOM	3921	CA	GLN	183	23.290	22.256	69.228	1.00	33.43	B
ATOM	3922	CB	GLN	183	22.261	23.284	69.688	1.00	36.19	B
ATOM	3923	CG	GLN	183	22.844	24.463	70.456	1.00	40.60	B
ATOM	3924	CD	GLN	183	21.781	25.458	70.916	1.00	43.17	B
ATOM	3925	OE1	GLN	183	20.902	25.122	71.711	1.00	45.10	B
ATOM	3926	NE2	GLN	183	21.856	26.687	70.408	1.00	42.17	B
ATOM	3927	C	GLN	183	22.513	21.122	68.578	1.00	30.84	B
ATOM	3928	O	GLN	183	22.098	21.224	67.436	1.00	29.43	B
ATOM	3929	N	MET	184	22.311	20.047	69.325	1.00	29.11	B
ATOM	3930	CA	MET	184	21.603	18.884	68.821	1.00	28.51	B
ATOM	3931	CB	MET	184	22.549	17.698	68.930	1.00	27.68	B
ATOM	3932	CG	MET	184	21.997	16.385	68.443	1.00	30.34	B
ATOM	3933	SD	MET	184	23.142	15.021	68.745	1.00	30.67	B
ATOM	3934	CE	MET	184	22.841	14.793	70.448	1.00	30.06	B
ATOM	3935	C	MET	184	20.298	18.650	69.595	1.00	29.09	B
ATOM	3936	O	MET	184	20.280	18.737	70.806	1.00	29.05	B
ATOM	3937	N	PHE	185	19.213	18.342	68.887	1.00	30.68	B
ATOM	3938	CA	PHE	185	17.921	18.112	69.537	1.00	31.83	B
ATOM	3939	CB	PHE	185	16.953	19.277	69.291	1.00	31.45	B
ATOM	3940	CG	PHE	185	17.520	20.626	69.637	1.00	30.24	B
ATOM	3941	CD1	PHE	185	18.381	21.275	68.763	1.00	29.12	B
ATOM	3942	CD2	PHE	185	17.215	21.234	70.850	1.00	28.98	B
ATOM	3943	CE1	PHE	185	18.929	22.500	69.082	1.00	28.97	B
ATOM	3944	CE2	PHE	185	17.762	22.461	71.180	1.00	29.87	B
ATOM	3945	CZ	PHE	185	18.624	23.098	70.289	1.00	29.79	B
ATOM	3946	C	PHE	185	17.236	16.883	68.976	1.00	33.71	B
ATOM	3947	O	PHE	185	17.473	16.515	67.845	1.00	33.43	B
ATOM	3948	N	ASP	186	16.393	16.245	69.782	1.00	37.53	B
ATOM	3949	CA	ASP	186	15.667	15.071	69.310	1.00	40.98	B
ATOM	3950	CB	ASP	186	14.857	14.413	70.431	1.00	43.17	B
ATOM	3951	CG	ASP	186	15.721	13.931	71.575	1.00	45.72	B
ATOM	3952	OD1	ASP	186	16.691	13.190	71.316	1.00	48.29	B
ATOM	3953	OD2	ASP	186	15.413	14.291	72.734	1.00	46.64	B
ATOM	3954	C	ASP	186	14.676	15.587	68.284	1.00	42.58	B
ATOM	3955	O	ASP	186	14.123	16.666	68.453	1.00	42.55	B
ATOM	3956	N	ASP	187	14.457	14.835	67.214	1.00	44.89	B
ATOM	3957	CA	ASP	187	13.528	15.287	66.188	1.00	46.96	B
ATOM	3958	CB	ASP	187	13.921	14.695	64.840	1.00	46.66	B
ATOM	3959	CG	ASP	187	13.090	15.232	63.718	1.00	46.68	B
ATOM	3960	OD1	ASP	187	13.381	14.891	62.555	1.00	47.95	B
ATOM	3961	OD2	ASP	187	12.144	15.996	64.008	1.00	45.37	B
ATOM	3962	C	ASP	187	12.127	14.881	66.604	1.00	48.78	B
ATOM	3963	O	ASP	187	11.844	13.696	66.773	1.00	49.04	B
ATOM	3964	N	PRO	188	11.235	15.870	66.799	1.00	50.85	B
ATOM	3965	CD	PRO	188	11.546	17.310	66.716	1.00	50.78	B
ATOM	3966	CA	PRO	188	9.838	15.660	67.209	1.00	52.07	B
ATOM	3967	CB	PRO	188	9.280	17.085	67.240	1.00	51.41	B
ATOM	3968	CG	PRO	188	10.496	17.916	67.605	1.00	50.84	B
ATOM	3969	C	PRO	188	9.071	14.705	66.302	1.00	53.79	B
ATOM	3970	O	PRO	188	8.249	13.900	66.753	1.00	52.56	B
ATOM	3971	N	ARG	189	9.340	14.817	65.011	1.00	56.26	B
ATOM	3972	CA	ARG	189	8.691	13.979	64.033	1.00	59.28	B
ATOM	3973	CB	ARG	189	9.218	14.349	62.649	1.00	60.03	B
ATOM	3974	CG	ARG	189	8.875	15.774	62.238	1.00	61.54	B
ATOM	3975	CD	ARG	189	9.366	16.081	60.833	1.00	62.62	B
ATOM	3976	NE	ARG	189	10.813	16.277	60.790	1.00	63.59	B
ATOM	3977	CZ	ARG	189	11.407	17.465	60.837	1.00	64.36	B
ATOM	3978	NH1	ARG	189	10.680	18.575	60.925	1.00	64.67	B
ATOM	3979	NH2	ARG	189	12.729	17.545	60.794	1.00	64.73	B
ATOM	3980	C	ARG	189	8.905	12.499	64.357	1.00	61.00	B
ATOM	3981	O	ARG	189	7.952	11.725	64.399	1.00	61.27	B
ATOM	3982	N	ASN	190	10.159	12.118	64.590	1.00	63.40	B
ATOM	3983	CA	ASN	190	10.516	10.735	64.914	1.00	65.21	B
ATOM	3984	CB	ASN	190	10.752	9.935	63.625	1.00	65.05	B
ATOM	3985	CG	ASN	190	11.750	10.604	62.692	1.00	64.67	B

ATOM	3986	OD1	ASN	190	12.954	10.474	62.861	1.00	64.77	B
ATOM	3987	ND2	ASN	190	11.242	11.332	61.707	1.00	63.52	B
ATOM	3988	C	ASN	190	11.757	10.684	65.807	1.00	66.41	B
ATOM	3989	O	ASN	190	12.850	11.038	65.381	1.00	66.57	B
ATOM	3990	N	LYS	191	11.575	10.241	67.051	1.00	67.89	B
ATOM	3991	CA	LYS	191	12.676	10.158	68.017	1.00	68.02	B
ATOM	3992	CB	LYS	191	12.151	9.687	69.378	1.00	69.77	B
ATOM	3993	CG	LYS	191	11.151	10.636	70.012	1.00	71.09	B
ATOM	3994	CD	LYS	191	11.787	11.982	70.297	1.00	72.77	B
ATOM	3995	CE	LYS	191	10.771	12.963	70.860	1.00	74.00	B
ATOM	3996	NZ	LYS	191	9.657	13.210	69.902	1.00	75.27	B
ATOM	3997	C	LYS	191	13.826	9.251	67.571	1.00	66.64	B
ATOM	3998	O	LYS	191	14.852	9.149	68.253	1.00	66.18	B
ATOM	3999	N	ARG	192	13.641	8.587	66.434	1.00	64.41	B
ATOM	4000	CA	ARG	192	14.668	7.720	65.878	1.00	62.32	B
ATOM	4001	CB	ARG	192	14.101	6.946	64.685	1.00	64.84	B
ATOM	4002	CG	ARG	192	15.134	6.138	63.909	1.00	68.49	B
ATOM	4003	CD	ARG	192	14.582	5.584	62.578	1.00	71.52	B
ATOM	4004	NE	ARG	192	14.312	6.616	61.569	1.00	73.79	B
ATOM	4005	CZ	ARG	192	13.207	7.359	61.506	1.00	74.82	B
ATOM	4006	NH1	ARG	192	12.232	7.201	62.393	1.00	75.36	B
ATOM	4007	NH2	ARG	192	13.079	8.275	60.555	1.00	75.53	B
ATOM	4008	C	ARG	192	15.822	8.612	65.403	1.00	59.33	B
ATOM	4009	O	ARG	192	16.991	8.235	65.479	1.00	58.48	B
ATOM	4010	N	GLY	193	15.468	9.805	64.927	1.00	55.93	B
ATOM	4011	CA	GLY	193	16.453	10.747	64.429	1.00	50.05	B
ATOM	4012	C	GLY	193	16.778	11.895	65.364	1.00	45.96	B
ATOM	4013	O	GLY	193	16.345	11.933	66.518	1.00	44.90	B
ATOM	4014	N	VAL	194	17.547	12.842	64.839	1.00	42.75	B
ATOM	4015	CA	VAL	194	17.968	14.006	65.596	1.00	39.18	B
ATOM	4016	CB	VAL	194	19.328	13.743	66.269	1.00	39.02	B
ATOM	4017	CG1	VAL	194	20.450	13.925	65.262	1.00	38.70	B
ATOM	4018	CG2	VAL	194	19.504	14.653	67.456	1.00	38.46	B
ATOM	4019	C	VAL	194	18.096	15.209	64.666	1.00	37.27	B
ATOM	4020	O	VAL	194	18.181	15.057	63.456	1.00	36.48	B
ATOM	4021	N	ILE	195	18.108	16.400	65.254	1.00	35.15	B
ATOM	4022	CA	ILE	195	18.230	17.645	64.501	1.00	33.17	B
ATOM	4023	CB	ILE	195	17.002	18.543	64.702	1.00	34.99	B
ATOM	4024	CG2	ILE	195	17.185	19.842	63.916	1.00	36.47	B
ATOM	4025	CG1	ILE	195	15.731	17.803	64.280	1.00	36.88	B
ATOM	4026	CD1	ILE	195	15.658	17.513	62.784	1.00	38.32	B
ATOM	4027	C	ILE	195	19.452	18.465	64.917	1.00	30.37	B
ATOM	4028	O	ILE	195	19.575	18.870	66.063	1.00	28.47	B
ATOM	4029	N	ILE	196	20.353	18.711	63.975	1.00	28.58	B
ATOM	4030	CA	ILE	196	21.538	19.503	64.270	1.00	27.51	B
ATOM	4031	CB	ILE	196	22.810	18.928	63.572	1.00	26.71	B
ATOM	4032	CG2	ILE	196	24.024	19.795	63.884	1.00	25.48	B
ATOM	4033	CG1	ILE	196	23.107	17.515	64.078	1.00	25.19	B
ATOM	4034	CD1	ILE	196	22.263	16.456	63.472	1.00	25.37	B
ATOM	4035	C	ILE	196	21.284	20.931	63.787	1.00	27.55	B
ATOM	4036	O	ILE	196	21.307	21.212	62.601	1.00	27.49	B
ATOM	4037	N	LYS	197	21.045	21.832	64.730	1.00	28.27	B
ATOM	4038	CA	LYS	197	20.765	23.229	64.418	1.00	27.24	B
ATOM	4039	CB	LYS	197	20.328	23.973	65.688	1.00	28.18	B
ATOM	4040	CG	LYS	197	19.970	25.451	65.508	1.00	26.93	B
ATOM	4041	CD	LYS	197	19.665	26.075	66.853	1.00	27.21	B
ATOM	4042	CE	LYS	197	19.417	27.563	66.750	1.00	26.28	B
ATOM	4043	NZ	LYS	197	19.153	28.144	68.104	1.00	26.63	B
ATOM	4044	C	LYS	197	21.961	23.947	63.821	1.00	26.61	B
ATOM	4045	O	LYS	197	23.039	23.974	64.406	1.00	27.65	B
ATOM	4046	N	GLY	198	21.762	24.513	62.637	1.00	26.31	B
ATOM	4047	CA	GLY	198	22.826	25.266	61.998	1.00	25.56	B
ATOM	4048	C	GLY	198	23.747	24.536	61.044	1.00	24.60	B
ATOM	4049	O	GLY	198	24.518	25.162	60.335	1.00	24.69	B
ATOM	4050	N	LEU	199	23.680	23.211	61.029	1.00	25.09	B
ATOM	4051	CA	LEU	199	24.523	22.433	60.130	1.00	25.50	B
ATOM	4052	CB	LEU	199	24.357	20.927	60.411	1.00	24.64	B
ATOM	4053	CG	LEU	199	25.219	19.950	59.597	1.00	24.37	B
ATOM	4054	CD1	LEU	199	26.699	20.274	59.742	1.00	22.90	B
ATOM	4055	CD2	LEU	199	24.942	18.535	60.068	1.00	23.77	B
ATOM	4056	C	LEU	199	24.235	22.767	58.648	1.00	25.50	B
ATOM	4057	O	LEU	199	23.160	22.510	58.114	1.00	24.77	B
ATOM	4058	N	GLU	200	25.225	23.350	57.991	1.00	26.00	B

ATOM	4059	CA	GLU	200	25.087	23.722	56.598	1.00	26.47	B
ATOM	4060	CB	GLU	200	26.274	24.568	56.143	1.00	27.75	B
ATOM	4061	CG	GLU	200	26.324	25.971	56.724	1.00	32.47	B
ATOM	4062	CD	GLU	200	25.112	26.821	56.339	1.00	35.25	B
ATOM	4063	OE1	GLU	200	24.061	26.700	57.004	1.00	38.07	B
ATOM	4064	OE2	GLU	200	25.196	27.600	55.363	1.00	35.41	B
ATOM	4065	C	GLU	200	25.029	22.508	55.686	1.00	27.12	B
ATOM	4066	O	GLU	200	25.586	21.457	55.972	1.00	26.69	B
ATOM	4067	N	GLU	201	24.327	22.678	54.579	1.00	27.51	B
ATOM	4068	CA	GLU	201	24.218	21.646	53.574	1.00	26.72	B
ATOM	4069	CB	GLU	201	22.790	21.135	53.468	1.00	27.33	B
ATOM	4070	CG	GLU	201	22.239	20.532	54.722	1.00	30.03	B
ATOM	4071	CD	GLU	201	20.954	19.773	54.457	1.00	32.95	B
ATOM	4072	OE1	GLU	201	20.075	19.784	55.345	1.00	34.01	B
ATOM	4073	OE2	GLU	201	20.817	19.167	53.367	1.00	33.38	B
ATOM	4074	C	GLU	201	24.581	22.363	52.278	1.00	26.18	B
ATOM	4075	O	GLU	201	23.866	23.259	51.853	1.00	25.94	B
ATOM	4076	N	ILE	202	25.707	21.996	51.674	1.00	25.78	B
ATOM	4077	CA	ILE	202	26.116	22.631	50.433	1.00	25.80	B
ATOM	4078	CB	ILE	202	27.636	22.813	50.360	1.00	25.61	B
ATOM	4079	CG2	ILE	202	28.022	23.102	48.914	1.00	25.19	B
ATOM	4080	CG1	ILE	202	28.089	23.969	51.258	1.00	26.32	B
ATOM	4081	CD1	ILE	202	27.704	23.871	52.722	1.00	25.98	B
ATOM	4082	C	ILE	202	25.655	21.820	49.231	1.00	26.76	B
ATOM	4083	O	ILE	202	25.798	20.597	49.195	1.00	26.87	B
ATOM	4084	N	THR	203	25.089	22.508	48.248	1.00	26.89	B
ATOM	4085	CA	THR	203	24.610	21.817	47.070	1.00	28.63	B
ATOM	4086	CB	THR	203	23.463	22.606	46.329	1.00	28.93	B
ATOM	4087	OG1	THR	203	22.297	22.683	47.167	1.00	28.96	B
ATOM	4088	CG2	THR	203	23.103	21.922	44.987	1.00	25.61	B
ATOM	4089	C	THR	203	25.774	21.634	46.120	1.00	29.69	B
ATOM	4090	O	THR	203	26.546	22.547	45.906	1.00	31.36	B
ATOM	4091	N	VAL	204	25.919	20.428	45.589	1.00	30.40	B
ATOM	4092	CA	VAL	204	26.967	20.168	44.620	1.00	30.44	B
ATOM	4093	CB	VAL	204	27.656	18.798	44.876	1.00	29.19	B
ATOM	4094	CG1	VAL	204	28.839	18.609	43.930	1.00	28.81	B
ATOM	4095	CG2	VAL	204	28.142	18.733	46.292	1.00	29.07	B
ATOM	4096	C	VAL	204	26.225	20.159	43.277	1.00	31.43	B
ATOM	4097	O	VAL	204	25.536	19.180	42.956	1.00	31.70	B
ATOM	4098	N	HIS	205	26.354	21.255	42.521	1.00	31.11	B
ATOM	4099	CA	HIS	205	25.709	21.420	41.214	1.00	30.37	B
ATOM	4100	CB	HIS	205	25.803	22.869	40.792	1.00	29.29	B
ATOM	4101	CG	HIS	205	25.131	23.788	41.747	1.00	29.35	B
ATOM	4102	CD2	HIS	205	25.631	24.594	42.712	1.00	29.07	B
ATOM	4103	ND1	HIS	205	23.760	23.890	41.831	1.00	29.17	B
ATOM	4104	CE1	HIS	205	23.444	24.721	42.806	1.00	29.14	B
ATOM	4105	NE2	HIS	205	24.561	25.161	43.357	1.00	29.64	B
ATOM	4106	C	HIS	205	26.252	20.533	40.100	1.00	30.88	B
ATOM	4107	O	HIS	205	25.508	20.130	39.216	1.00	31.82	B
ATOM	4108	N	ASN	206	27.544	20.238	40.138	1.00	29.74	B
ATOM	4109	CA	ASN	206	28.127	19.370	39.141	1.00	29.11	B
ATOM	4110	CB	ASN	206	28.377	20.158	37.852	1.00	28.48	B
ATOM	4111	CG	ASN	206	29.156	21.438	38.091	1.00	29.29	B
ATOM	4112	OD1	ASN	206	30.252	21.412	38.645	1.00	28.71	B
ATOM	4113	ND2	ASN	206	28.594	22.562	37.673	1.00	28.54	B
ATOM	4114	C	ASN	206	29.387	18.760	39.729	1.00	28.47	B
ATOM	4115	O	ASN	206	29.740	19.032	40.852	1.00	27.98	B
ATOM	4116	N	LYS	207	30.063	17.924	38.957	1.00	29.11	B
ATOM	4117	CA	LYS	207	31.274	17.291	39.445	1.00	30.00	B
ATOM	4118	CB	LYS	207	31.662	16.107	38.553	1.00	30.11	B
ATOM	4119	CG	LYS	207	32.257	16.495	37.222	1.00	32.75	B
ATOM	4120	CD	LYS	207	32.719	15.270	36.441	1.00	33.95	B
ATOM	4121	CE	LYS	207	33.466	15.669	35.164	1.00	34.56	B
ATOM	4122	NZ	LYS	207	34.775	16.370	35.404	1.00	33.30	B
ATOM	4123	C	LYS	207	32.425	18.293	39.488	1.00	30.73	B
ATOM	4124	O	LYS	207	33.458	18.026	40.089	1.00	32.12	B
ATOM	4125	N	ASP	208	32.241	19.451	38.863	1.00	29.02	B
ATOM	4126	CA	ASP	208	33.301	20.453	38.850	1.00	28.26	B
ATOM	4127	CB	ASP	208	33.234	21.261	37.556	1.00	31.08	B
ATOM	4128	CG	ASP	208	33.702	20.463	36.354	1.00	32.65	B
ATOM	4129	OD1	ASP	208	33.221	20.729	35.233	1.00	33.84	B
ATOM	4130	OD2	ASP	208	34.567	19.570	36.523	1.00	33.75	B
ATOM	4131	C	ASP	208	33.277	21.374	40.065	1.00	26.42	B

ATOM	4132	O	ASP	208	33.989	22.372	40.117	1.00	24.98	B
ATOM	4133	N	GLU	209	32.462	21.032	41.052	1.00	25.24	B
ATOM	4134	CA	GLU	209	32.388	21.831	42.272	1.00	25.22	B
ATOM	4135	CB	GLU	209	30.958	22.278	42.595	1.00	27.01	B
ATOM	4136	CG	GLU	209	30.306	23.237	41.602	1.00	30.48	B
ATOM	4137	CD	GLU	209	29.069	23.926	42.167	1.00	32.55	B
ATOM	4138	OE1	GLU	209	28.371	24.610	41.385	1.00	34.80	B
ATOM	4139	OE2	GLU	209	28.804	23.793	43.382	1.00	33.17	B
ATOM	4140	C	GLU	209	32.832	21.030	43.490	1.00	24.23	B
ATOM	4141	O	GLU	209	33.194	21.596	44.513	1.00	25.15	B
ATOM	4142	N	VAL	210	32.835	19.708	43.373	1.00	21.99	B
ATOM	4143	CA	VAL	210	33.205	18.882	44.514	1.00	18.98	B
ATOM	4144	CB	VAL	210	32.987	17.360	44.217	1.00	17.62	B
ATOM	4145	CG1	VAL	210	32.238	17.180	42.928	1.00	17.92	B
ATOM	4146	CG2	VAL	210	34.290	16.638	44.159	1.00	17.49	B
ATOM	4147	C	VAL	210	34.609	19.093	45.082	1.00	18.13	B
ATOM	4148	O	VAL	210	34.775	19.138	46.289	1.00	19.29	B
ATOM	4149	N	TYR	211	35.620	19.238	44.232	1.00	17.72	B
ATOM	4150	CA	TYR	211	36.968	19.401	44.770	1.00	15.84	B
ATOM	4151	CB	TYR	211	38.030	19.361	43.656	1.00	14.23	B
ATOM	4152	CG	TYR	211	39.441	19.224	44.196	1.00	13.57	B
ATOM	4153	CD1	TYR	211	39.807	18.110	44.937	1.00	12.81	B
ATOM	4154	CE1	TYR	211	41.062	18.018	45.528	1.00	12.54	B
ATOM	4155	CD2	TYR	211	40.379	20.246	44.048	1.00	14.65	B
ATOM	4156	CE2	TYR	211	41.651	20.166	44.642	1.00	13.74	B
ATOM	4157	CZ	TYR	211	41.987	19.048	45.386	1.00	14.45	B
ATOM	4158	OH	TYR	211	43.235	18.972	45.997	1.00	10.15	B
ATOM	4159	C	TYR	211	37.083	20.665	45.608	1.00	15.70	B
ATOM	4160	O	TYR	211	37.626	20.620	46.696	1.00	14.92	B
ATOM	4161	N	GLN	212	36.557	21.781	45.101	1.00	17.75	B
ATOM	4162	CA	GLN	212	36.582	23.064	45.819	1.00	18.64	B
ATOM	4163	CB	GLN	212	35.897	24.154	44.983	1.00	19.40	B
ATOM	4164	CG	GLN	212	35.962	25.543	45.607	1.00	24.51	B
ATOM	4165	CD	GLN	212	35.764	26.672	44.587	1.00	26.82	B
ATOM	4166	OE1	GLN	212	35.046	26.508	43.594	1.00	25.33	B
ATOM	4167	NE2	GLN	212	36.391	27.832	44.844	1.00	26.86	B
ATOM	4168	C	GLN	212	35.909	22.923	47.192	1.00	18.53	B
ATOM	4169	O	GLN	212	36.420	23.374	48.193	1.00	19.69	B
ATOM	4170	N	ILE	213	34.759	22.265	47.230	1.00	19.83	B
ATOM	4171	CA	ILE	213	34.031	22.048	48.485	1.00	19.97	B
ATOM	4172	CB	ILE	213	32.664	21.350	48.237	1.00	20.59	B
ATOM	4173	CG2	ILE	213	32.022	20.933	49.579	1.00	19.77	B
ATOM	4174	CG1	ILE	213	31.758	22.285	47.441	1.00	20.66	B
ATOM	4175	CD1	ILE	213	30.505	21.626	46.928	1.00	22.87	B
ATOM	4176	C	ILE	213	34.831	21.189	49.461	1.00	20.10	B
ATOM	4177	O	ILE	213	34.822	21.446	50.672	1.00	20.46	B
ATOM	4178	N	LEU	214	35.489	20.156	48.937	1.00	19.00	B
ATOM	4179	CA	LEU	214	36.310	19.282	49.759	1.00	18.96	B
ATOM	4180	CB	LEU	214	36.829	18.100	48.950	1.00	18.27	B
ATOM	4181	CG	LEU	214	36.013	16.826	49.015	1.00	18.28	B
ATOM	4182	CD1	LEU	214	34.547	17.179	48.926	1.00	22.38	B
ATOM	4183	CD2	LEU	214	36.443	15.908	47.895	1.00	17.95	B
ATOM	4184	C	LEU	214	37.507	20.048	50.316	1.00	19.17	B
ATOM	4185	O	LEU	214	37.920	19.821	51.443	1.00	20.21	B
ATOM	4186	N	GLU	215	38.055	20.967	49.523	1.00	19.88	B
ATOM	4187	CA	GLU	215	39.208	21.768	49.953	1.00	19.18	B
ATOM	4188	CB	GLU	215	39.748	22.628	48.797	1.00	19.26	B
ATOM	4189	CG	GLU	215	40.496	21.863	47.699	1.00	20.08	B
ATOM	4190	CD	GLU	215	41.103	22.786	46.630	1.00	20.78	B
ATOM	4191	OE1	GLU	215	42.352	22.898	46.580	1.00	16.87	B
ATOM	4192	OE2	GLU	215	40.337	23.399	45.842	1.00	19.38	B
ATOM	4193	C	GLU	215	38.855	22.700	51.110	1.00	18.78	B
ATOM	4194	O	GLU	215	39.592	22.798	52.092	1.00	17.36	B
ATOM	4195	N	LYS	216	37.732	23.397	50.988	1.00	19.53	B
ATOM	4196	CA	LYS	216	37.293	24.300	52.042	1.00	20.63	B
ATOM	4197	CB	LYS	216	35.993	24.988	51.620	1.00	22.77	B
ATOM	4198	CG	LYS	216	36.240	26.094	50.602	1.00	29.39	B
ATOM	4199	CD	LYS	216	34.962	26.743	50.069	1.00	33.26	B
ATOM	4200	CE	LYS	216	35.281	27.963	49.187	1.00	35.91	B
ATOM	4201	NZ	LYS	216	36.198	27.671	48.028	1.00	37.67	B
ATOM	4202	C	LYS	216	37.144	23.547	53.361	1.00	20.03	B
ATOM	4203	O	LYS	216	37.501	24.057	54.416	1.00	21.40	B
ATOM	4204	N	GLY	217	36.628	22.329	53.309	1.00	18.86	B

ATOM	4205	CA	GLY	217	36.492	21.587	54.543	1.00	18.29	B
ATOM	4206	C	GLY	217	37.869	21.334	55.128	1.00	18.39	B
ATOM	4207	O	GLY	217	38.103	21.531	56.307	1.00	18.74	B
ATOM	4208	N	ALA	218	38.792	20.895	54.282	1.00	19.27	B
ATOM	4209	CA	ALA	218	40.148	20.607	54.737	1.00	19.03	B
ATOM	4210	CB	ALA	218	40.996	20.061	53.580	1.00	18.52	B
ATOM	4211	C	ALA	218	40.827	21.818	55.363	1.00	18.17	B
ATOM	4212	O	ALA	218	41.470	21.706	56.403	1.00	19.12	B
ATOM	4213	N	ALA	219	40.691	22.980	54.735	1.00	17.99	B
ATOM	4214	CA	ALA	219	41.315	24.203	55.266	1.00	16.17	B
ATOM	4215	CB	ALA	219	41.044	25.404	54.323	1.00	14.07	B
ATOM	4216	C	ALA	219	40.792	24.505	56.671	1.00	14.78	B
ATOM	4217	O	ALA	219	41.552	24.760	57.599	1.00	15.56	B
ATOM	4218	N	LYS	220	39.479	24.450	56.823	1.00	14.00	B
ATOM	4219	CA	LYS	220	38.859	24.729	58.110	1.00	13.80	B
ATOM	4220	CB	LYS	220	37.338	24.667	57.978	1.00	11.84	B
ATOM	4221	CG	LYS	220	36.603	25.222	59.177	1.00	12.63	B
ATOM	4222	CD	LYS	220	35.130	25.462	58.884	1.00	11.67	B
ATOM	4223	CE	LYS	220	34.464	26.087	60.092	1.00	13.88	B
ATOM	4224	NZ	LYS	220	32.993	26.287	59.939	1.00	12.51	B
ATOM	4225	C	LYS	220	39.303	23.734	59.173	1.00	14.26	B
ATOM	4226	O	LYS	220	39.442	24.067	60.350	1.00	15.25	B
ATOM	4227	N	ARG	221	39.513	22.498	58.748	1.00	14.19	B
ATOM	4228	CA	ARG	221	39.936	21.438	59.647	1.00	11.64	B
ATOM	4229	CB	ARG	221	39.878	20.111	58.889	1.00	13.12	B
ATOM	4230	CG	ARG	221	40.038	18.857	59.751	1.00	13.06	B
ATOM	4231	CD	ARG	221	39.999	17.586	58.902	1.00	11.48	B
ATOM	4232	NE	ARG	221	38.638	17.093	58.691	1.00	8.87	B
ATOM	4233	CZ	ARG	221	38.317	16.184	57.774	1.00	8.38	B
ATOM	4234	NH1	ARG	221	39.255	15.687	56.976	1.00	5.16	B
ATOM	4235	NH2	ARG	221	37.074	15.732	57.687	1.00	8.15	B
ATOM	4236	C	ARG	221	41.345	21.737	60.174	1.00	10.67	B
ATOM	4237	O	ARG	221	41.686	21.394	61.314	1.00	10.15	B
ATOM	4238	N	THR	222	42.167	22.372	59.342	1.00	10.52	B
ATOM	4239	CA	THR	222	43.515	22.747	59.752	1.00	7.37	B
ATOM	4240	CB	THR	222	44.277	23.438	58.634	1.00	6.75	B
ATOM	4241	OG1	THR	222	44.586	22.466	57.637	1.00	9.09	B
ATOM	4242	CG2	THR	222	45.573	24.026	59.136	1.00	5.92	B
ATOM	4243	C	THR	222	43.475	23.692	60.916	1.00	5.52	B
ATOM	4244	O	THR	222	44.265	23.598	61.797	1.00	6.41	B
ATOM	4245	N	THR	223	42.527	24.607	60.906	1.00	5.73	B
ATOM	4246	CA	THR	223	42.443	25.550	61.990	1.00	7.41	B
ATOM	4247	CB	THR	223	41.481	26.706	61.654	1.00	9.80	B
ATOM	4248	OG1	THR	223	40.126	26.260	61.807	1.00	13.96	B
ATOM	4249	CG2	THR	223	41.716	27.205	60.212	1.00	11.03	B
ATOM	4250	C	THR	223	41.941	24.801	63.206	1.00	8.79	B
ATOM	4251	O	THR	223	42.353	25.101	64.337	1.00	11.00	B
ATOM	4252	N	ALA	224	41.093	23.796	62.970	1.00	9.46	B
ATOM	4253	CA	ALA	224	40.537	23.001	64.069	1.00	9.41	B
ATOM	4254	CB	ALA	224	39.514	21.966	63.570	1.00	8.72	B
ATOM	4255	C	ALA	224	41.645	22.288	64.798	1.00	10.87	B
ATOM	4256	O	ALA	224	41.693	22.258	66.041	1.00	10.92	B
ATOM	4257	N	ALA	225	42.526	21.678	64.020	1.00	11.03	B
ATOM	4258	CA	ALA	225	43.647	20.977	64.608	1.00	10.24	B
ATOM	4259	CB	ALA	225	44.484	20.347	63.517	1.00	9.24	B
ATOM	4260	C	ALA	225	44.502	21.942	65.446	1.00	11.63	B
ATOM	4261	O	ALA	225	44.983	21.592	66.516	1.00	12.58	B
ATOM	4262	N	THR	226	44.676	23.164	64.957	1.00	13.45	B
ATOM	4263	CA	THR	226	45.490	24.156	65.650	1.00	15.18	B
ATOM	4264	CB	THR	226	45.557	25.470	64.868	1.00	14.69	B
ATOM	4265	OG1	THR	226	46.323	25.286	63.670	1.00	16.29	B
ATOM	4266	CG2	THR	226	46.186	26.534	65.716	1.00	15.17	B
ATOM	4267	C	THR	226	44.901	24.452	67.007	1.00	16.64	B
ATOM	4268	O	THR	226	45.617	24.553	67.998	1.00	16.41	B
ATOM	4269	N	LEU	227	43.575	24.575	67.025	1.00	18.18	B
ATOM	4270	CA	LEU	227	42.805	24.875	68.238	1.00	18.74	B
ATOM	4271	CB	LEU	227	41.367	25.310	67.899	1.00	19.87	B
ATOM	4272	CG	LEU	227	40.955	26.772	68.051	1.00	21.86	B
ATOM	4273	CD1	LEU	227	41.103	27.134	69.518	1.00	21.93	B
ATOM	4274	CD2	LEU	227	41.786	27.693	67.155	1.00	21.51	B
ATOM	4275	C	LEU	227	42.651	23.733	69.239	1.00	18.17	B
ATOM	4276	O	LEU	227	42.783	23.928	70.435	1.00	18.61	B
ATOM	4277	N	MET	228	42.380	22.536	68.742	1.00	18.27	B

ATOM	4278	CA	MET	228	42.160	21.404	69.634	1.00	17.51	B
ATOM	4279	CB	MET	228	40.800	20.772	69.302	1.00	16.30	B
ATOM	4280	CG	MET	228	39.649	21.745	69.495	1.00	16.20	B
ATOM	4281	SD	MET	228	38.056	21.201	68.874	1.00	19.18	B
ATOM	4282	CE	MET	228	38.092	22.153	67.250	1.00	17.21	B
ATOM	4283	C	MET	228	43.250	20.342	69.614	1.00	18.14	B
ATOM	4284	O	MET	228	43.769	19.990	68.549	1.00	20.11	B
ATOM	4285	N	ASN	229	43.571	19.834	70.807	1.00	16.66	B
ATOM	4286	CA	ASN	229	44.589	18.799	70.992	1.00	16.35	B
ATOM	4287	CB	ASN	229	44.824	18.543	72.485	1.00	15.94	B
ATOM	4288	CG	ASN	229	45.350	19.764	73.209	1.00	16.33	B
ATOM	4289	OD1	ASN	229	45.764	20.739	72.588	1.00	17.78	B
ATOM	4290	ND2	ASN	229	45.340	19.711	74.534	1.00	14.68	B
ATOM	4291	C	ASN	229	44.311	17.448	70.313	1.00	15.68	B
ATOM	4292	O	ASN	229	43.228	16.873	70.460	1.00	15.38	B
ATOM	4293	N	ALA	230	45.300	16.950	69.569	1.00	14.15	B
ATOM	4294	CA	ALA	230	45.171	15.679	68.863	1.00	12.00	B
ATOM	4295	CB	ALA	230	45.241	14.546	69.847	1.00	11.64	B
ATOM	4296	C	ALA	230	43.869	15.595	68.079	1.00	11.58	B
ATOM	4297	O	ALA	230	43.269	14.519	67.977	1.00	10.16	B
ATOM	4298	N	TYR	231	43.443	16.725	67.519	1.00	11.27	B
ATOM	4299	CA	TYR	231	42.200	16.775	66.761	1.00	12.69	B
ATOM	4300	CB	TYR	231	42.047	18.119	66.029	1.00	11.10	B
ATOM	4301	CG	TYR	231	40.667	18.312	65.435	1.00	10.24	B
ATOM	4302	CD1	TYR	231	40.404	17.998	64.112	1.00	9.88	B
ATOM	4303	CE1	TYR	231	39.121	18.122	63.598	1.00	10.11	B
ATOM	4304	CD2	TYR	231	39.606	18.760	66.229	1.00	11.37	B
ATOM	4305	CE2	TYR	231	38.316	18.886	65.716	1.00	10.13	B
ATOM	4306	CZ	TYR	231	38.079	18.559	64.402	1.00	9.90	B
ATOM	4307	OH	TYR	231	36.780	18.623	63.936	1.00	7.41	B
ATOM	4308	C	TYR	231	41.988	15.645	65.748	1.00	13.47	B
ATOM	4309	O	TYR	231	41.016	14.916	65.837	1.00	14.47	B
ATOM	4310	N	SER	232	42.904	15.481	64.800	1.00	15.55	B
ATOM	4311	CA	SER	232	42.744	14.446	63.777	1.00	15.70	B
ATOM	4312	CB	SER	232	43.907	14.490	62.779	1.00	17.08	B
ATOM	4313	OG	SER	232	45.145	14.290	63.419	1.00	20.92	B
ATOM	4314	C	SER	232	42.608	13.020	64.308	1.00	15.28	B
ATOM	4315	O	SER	232	41.898	12.203	63.726	1.00	16.22	B
ATOM	4316	N	SER	233	43.260	12.711	65.417	1.00	12.45	B
ATOM	4317	CA	SER	233	43.173	11.352	65.919	1.00	12.60	B
ATOM	4318	CB	SER	233	44.477	10.942	66.596	1.00	13.54	B
ATOM	4319	OG	SER	233	44.662	11.602	67.838	1.00	15.82	B
ATOM	4320	C	SER	233	42.057	11.167	66.921	1.00	12.47	B
ATOM	4321	O	SER	233	41.604	10.047	67.155	1.00	12.18	B
ATOM	4322	N	ARG	234	41.612	12.265	67.523	1.00	11.28	B
ATOM	4323	CA	ARG	234	40.558	12.168	68.532	1.00	9.69	B
ATOM	4324	CB	ARG	234	40.919	12.961	69.784	1.00	10.96	B
ATOM	4325	CG	ARG	234	41.315	12.112	70.975	1.00	13.22	B
ATOM	4326	CD	ARG	234	42.707	12.435	71.494	1.00	16.77	B
ATOM	4327	NE	ARG	234	42.755	13.676	72.263	1.00	20.42	B
ATOM	4328	CZ	ARG	234	43.751	14.005	73.083	1.00	22.86	B
ATOM	4329	NH1	ARG	234	44.791	13.186	73.242	1.00	22.37	B
ATOM	4330	NH2	ARG	234	43.690	15.140	73.767	1.00	25.64	B
ATOM	4331	C	ARG	234	39.168	12.617	68.118	1.00	7.73	B
ATOM	4332	O	ARG	234	38.258	12.599	68.924	1.00	8.22	B
ATOM	4333	N	SER	235	39.006	13.014	66.862	1.00	6.52	B
ATOM	4334	CA	SER	235	37.697	13.455	66.394	1.00	4.31	B
ATOM	4335	CB	SER	235	37.785	14.801	65.647	1.00	2.24	B
ATOM	4336	OG	SER	235	38.745	14.780	64.602	1.00	1.00	B
ATOM	4337	C	SER	235	37.048	12.437	65.488	1.00	2.58	B
ATOM	4338	O	SER	235	37.704	11.648	64.854	1.00	3.58	B
ATOM	4339	N	HIS	236	35.725	12.465	65.472	1.00	4.87	B
ATOM	4340	CA	HIS	236	34.911	11.587	64.631	1.00	5.05	B
ATOM	4341	CB	HIS	236	33.691	11.087	65.386	1.00	4.65	B
ATOM	4342	CG	HIS	236	34.032	10.280	66.586	1.00	4.01	B
ATOM	4343	CD2	HIS	236	34.066	10.607	67.899	1.00	3.63	B
ATOM	4344	ND1	HIS	236	34.437	8.965	66.504	1.00	3.84	B
ATOM	4345	CE1	HIS	236	34.704	8.517	67.717	1.00	4.48	B
ATOM	4346	NE2	HIS	236	34.487	9.494	68.582	1.00	4.72	B
ATOM	4347	C	HIS	236	34.347	12.498	63.556	1.00	6.99	B
ATOM	4348	O	HIS	236	33.810	13.556	63.878	1.00	9.70	B
ATOM	4349	N	SER	237	34.475	12.108	62.291	1.00	7.23	B
ATOM	4350	CA	SER	237	33.951	12.933	61.208	1.00	6.69	B

ATOM	4351	CB	SER	237	35.058	13.406	60.253	1.00	5.37	B	
ATOM	4352	OG	SER	237	35.464	12.358	59.380	1.00	3.60	B	
ATOM	4353	C	SER	237	32.946	12.157	60.393	1.00	7.89	B	
ATOM	4354	O	SER	237	33.196	11.040	59.976	1.00	9.95	B	
ATOM	4355	N	VAL	238	31.787	12.753	60.180	1.00	7.91	B	
ATOM	4356	CA	VAL	238	30.787	12.078	59.392	1.00	7.74	B	
ATOM	4357	CB	VAL	238	29.560	11.740	60.282	1.00	8.04	B	
ATOM	4358	CG1	VAL	238	29.413	12.787	61.328	1.00	7.80	B	
ATOM	4359	CG2	VAL	238	28.307	11.669	59.460	1.00	8.71	B	
ATOM	4360	C	VAL	238	30.421	12.935	58.182	1.00	8.25	B	
ATOM	4361	O	VAL	238	29.776	13.952	58.323	1.00	9.09	B	
ATOM	4362	N	PHE	239	30.883	12.511	57.002	1.00	8.31	B	
ATOM	4363	CA	PHE	239	30.609	13.198	55.732	1.00	8.81	B	
ATOM	4364	CB	PHE	239	31.793	13.036	54.759	1.00	6.73	B	
ATOM	4365	CG	PHE	239	31.693	13.893	53.525	1.00	6.12	B	
ATOM	4366	CD1	PHE	239	30.815	13.557	52.500	1.00	5.69	B	
ATOM	4367	CD2	PHE	239	32.462	15.046	53.394	1.00	5.95	B	
ATOM	4368	CE1	PHE	239	30.705	14.364	51.348	1.00	5.30	B	
ATOM	4369	CE2	PHE	239	32.354	15.854	52.247	1.00	5.11	B	
ATOM	4370	CZ	PHE	239	31.475	15.511	51.224	1.00	3.58	B	
ATOM	4371	C	PHE	239	29.350	12.553	55.148	1.00	9.90	B	
ATOM	4372	O	PHE	239	29.327	11.356	54.859	1.00	9.81	B	
ATOM	4373	N	SER	240	28.305	13.359	54.982	1.00	10.63	B	
ATOM	4374	CA	SER	240	27.039	12.871	54.466	1.00	9.05	B	
ATOM	4375	CB	SER	240	25.926	13.194	55.467	1.00	9.24	B	
ATOM	4376	OG	SER	240	26.182	12.631	56.742	1.00	8.98	B	
ATOM	4377	C	SER	240	26.678	13.462	53.105	1.00	10.23	B	
ATOM	4378	O	SER	240	26.809	14.668	52.877	1.00	10.82	B	
ATOM	4379	N	VAL	241	26.230	12.601	52.198	1.00	10.77	B	
ATOM	4380	CA	VAL	241	25.813	13.044	50.874	1.00	12.14	B	
ATOM	4381	CB	VAL	241	26.748	12.492	49.775	1.00	12.12	B	
ATOM	4382	CG1	VAL	241	26.981	11.008	50.002	1.00	13.27	B	
ATOM	4383	CG2	VAL	241	26.143	12.736	48.394	1.00	11.17	B	
ATOM	4384	C	VAL	241	24.379	12.565	50.649	1.00	13.61	B	
ATOM	4385	O	VAL	241	24.092	11.365	50.700	1.00	13.01	B	
ATOM	4386	N	THR	242	23.478	13.513	50.422	1.00	14.36	B	
ATOM	4387	CA	THR	242	22.078	13.203	50.217	1.00	16.18	B	
ATOM	4388	CB	THR	242	21.198	14.104	51.118	1.00	17.52	B	
ATOM	4389	OG1	THR	242	21.546	13.897	52.496	1.00	19.73	B	
ATOM	4390	CG2	THR	242	19.738	13.766	50.954	1.00	20.46	B	
ATOM	4391	C	THR	242	21.746	13.418	48.741	1.00	18.15	B	
ATOM	4392	O	THR	242	22.212	14.357	48.128	1.00	19.20	B	
ATOM	4393	N	ILE	243	20.945	12.521	48.180	1.00	20.44	B	
ATOM	4394	CA	ILE	243	20.560	12.619	46.785	1.00	23.13	B	
ATOM	4395	CB	ILE	243	21.178	11.477	45.941	1.00	22.27	B	
ATOM	4396	CG2	ILE	243	20.962	11.770	44.475	1.00	18.06	B	
ATOM	4397	CG1	ILE	243	22.663	11.310	46.270	1.00	21.29	B	
ATOM	4398	CD1	ILE	243	23.247	10.072	45.722	1.00	21.09	B	
ATOM	4399	C	ILE	243	19.043	12.555	46.628	1.00	26.42	B	
ATOM	4400	O	ILE	243	18.442	11.488	46.790	1.00	27.92	B	
ATOM	4401	N	HIS	244	18.437	13.707	46.340	1.00	29.29	B	
ATOM	4402	CA	HIS	244	17.001	13.808	46.117	1.00	30.50	B	
ATOM	4403	CB	HIS	244	16.486	15.226	46.393	1.00	31.87	B	
ATOM	4404	CG	HIS	244	16.375	15.565	47.845	1.00	34.67	B	
ATOM	4405	CD2	HIS	244	15.341	15.441	48.712	1.00	35.28	B	
ATOM	4406	ND1	HIS	244	17.424	16.087	48.577	1.00	36.67	B	
ATOM	4407	CE1	HIS	244	17.040	16.267	49.828	1.00	35.69	B	
ATOM	4408	NE2	HIS	244	15.778	15.881	49.936	1.00	35.59	B	
ATOM	4409	C	HIS	244	16.803	13.494	44.637	1.00	32.12	B	
ATOM	4410	O	HIS	244	17.277	14.228	43.755	1.00	32.44	B	
ATOM	4411	N	MET	245	16.122	12.388	44.368	1.00	32.37	B	
ATOM	4412	CA	MET	245	15.877	11.968	42.998	1.00	32.37	B	
ATOM	4413	CB	MET	245	16.475	10.578	42.791	1.00	31.86	B	
ATOM	4414	CG	MET	245	17.968	10.548	43.055	1.00	31.73	B	
ATOM	4415	SD	MET	245	18.589	8.875	43.225	1.00	33.02	B	
ATOM	4416	CE	MET	245	18.034	8.477	44.892	1.00	31.10	B	
ATOM	4417	C	MET	245	14.401	12.002	42.601	1.00	31.83	B	
ATOM	4418	O	MET	245	13.509	11.738	43.415	1.00	31.92	B	
ATOM	4419	N	LYS	246	14.159	12.334	41.337	1.00	31.84	B	
ATOM	4420	CA	LYS	246	12.811	12.428	40.804	1.00	31.99	B	
ATOM	4421	CB	LYS	246	12.350	13.895	40.781	1.00	32.10	B	
ATOM	4422	CG	LYS	246	10.922	14.087	40.292	1.00	34.26	B	
ATOM	4423	CD	LYS	246	10.606	15.539	39.946	1.00	34.52	B	

ATOM	4424	CE	LYS	246	10.646	16.433	41.173	1.00	36.15	B	
ATOM	4425	NZ	LYS	246	10.457	17.872	40.836	1.00	35.42	B	
ATOM	4426	C	LYS	246	12.761	11.870	39.382	1.00	31.58	B	
ATOM	4427	O	LYS	246	13.439	12.358	38.480	1.00	30.24	B	
ATOM	4428	N	GLU	247	11.967	10.824	39.196	1.00	31.71	B	
ATOM	4429	CA	GLU	247	11.808	10.238	37.874	1.00	30.99	B	
ATOM	4430	CB	GLU	247	12.337	8.801	37.855	1.00	32.21	B	
ATOM	4431	CG	GLU	247	11.815	7.897	38.961	1.00	33.61	B	
ATOM	4432	CD	GLU	247	12.672	6.647	39.115	1.00	35.27	B	
ATOM	4433	OE1	GLU	247	12.420	5.841	40.037	1.00	35.63	B	
ATOM	4434	OE2	GLU	247	13.609	6.469	38.307	1.00	35.39	B	
ATOM	4435	C	GLU	247	10.338	10.298	37.479	1.00	30.04	B	
ATOM	4436	O	GLU	247	9.448	10.169	38.317	1.00	29.68	B	
ATOM	4437	N	THR	248	10.083	10.513	36.197	1.00	28.13	B	
ATOM	4438	CA	THR	248	8.716	10.591	35.720	1.00	26.83	B	
ATOM	4439	CB	THR	248	8.506	11.895	34.942	1.00	25.80	B	
ATOM	4440	OG1	THR	248	8.937	12.995	35.750	1.00	24.67	B	
ATOM	4441	CG2	THR	248	7.046	12.096	34.617	1.00	25.62	B	
ATOM	4442	C	THR	248	8.406	9.395	34.822	1.00	26.77	B	
ATOM	4443	O	THR	248	9.168	9.077	33.914	1.00	27.38	B	
ATOM	4444	N	THR	249	7.288	8.732	35.092	1.00	26.76	B	
ATOM	4445	CA	THR	249	6.877	7.580	34.302	1.00	26.72	B	
ATOM	4446	CB	THR	249	5.759	6.784	35.011	1.00	26.45	B	
ATOM	4447	OG1	THR	249	4.575	7.587	35.088	1.00	27.92	B	
ATOM	4448	CG2	THR	249	6.180	6.404	36.423	1.00	25.26	B	
ATOM	4449	C	THR	249	6.353	8.040	32.938	1.00	27.55	B	
ATOM	4450	O	THR	249	6.316	9.226	32.638	1.00	27.26	B	
ATOM	4451	N	ILE	250	5.956	7.078	32.113	1.00	29.51	B	
ATOM	4452	CA	ILE	250	5.434	7.353	30.774	1.00	30.16	B	
ATOM	4453	CB	ILE	250	5.444	6.074	29.901	1.00	29.03	B	
ATOM	4454	CG2	ILE	250	4.410	5.082	30.421	1.00	27.86	B	
ATOM	4455	CG1	ILE	250	5.157	6.431	28.443	1.00	28.33	B	
ATOM	4456	CD1	ILE	250	5.425	5.295	27.476	1.00	26.91	B	
ATOM	4457	C	ILE	250	4.005	7.884	30.877	1.00	31.97	B	
ATOM	4458	O	ILE	250	3.400	8.286	29.891	1.00	31.50	B	
ATOM	4459	N	ASP	251	3.477	7.875	32.095	1.00	34.02	B	
ATOM	4460	CA	ASP	251	2.132	8.368	32.359	1.00	36.26	B	
ATOM	4461	CB	ASP	251	1.425	7.469	33.381	1.00	36.12	B	
ATOM	4462	CG	ASP	251	0.789	6.242	32.750	1.00	36.40	B	
ATOM	4463	OD1	ASP	251	0.223	5.420	33.509	1.00	34.19	B	
ATOM	4464	OD2	ASP	251	0.854	6.119	31.504	1.00	36.03	B	
ATOM	4465	C	ASP	251	2.164	9.804	32.910	1.00	37.47	B	
ATOM	4466	O	ASP	251	1.140	10.468	32.990	1.00	38.11	B	
ATOM	4467	N	GLY	252	3.350	10.273	33.284	1.00	37.77	B	
ATOM	4468	CA	GLY	252	3.471	11.613	33.822	1.00	37.41	B	
ATOM	4469	C	GLY	252	3.566	11.662	35.338	1.00	38.71	B	
ATOM	4470	O	GLY	252	3.747	12.734	35.912	1.00	38.78	B	
ATOM	4471	N	GLU	253	3.440	10.516	36.003	1.00	38.85	B	
ATOM	4472	CA	GLU	253	3.533	10.511	37.459	1.00	39.67	B	
ATOM	4473	CB	GLU	253	3.020	9.200	38.052	1.00	41.37	B	
ATOM	4474	CG	GLU	253	3.181	9.143	39.573	1.00	43.75	B	
ATOM	4475	CD	GLU	253	2.814	7.803	40.188	1.00	44.31	B	
ATOM	4476	OE1	GLU	253	3.083	7.612	41.398	1.00	44.42	B	
ATOM	4477	OE2	GLU	253	2.256	6.945	39.470	1.00	45.10	B	
ATOM	4478	C	GLU	253	4.988	10.668	37.883	1.00	39.49	B	
ATOM	4479	O	GLU	253	5.890	10.286	37.149	1.00	39.20	B	
ATOM	4480	N	GLU	254	5.210	11.239	39.064	1.00	39.27	B	
ATOM	4481	CA	GLU	254	6.568	11.426	39.567	1.00	40.50	B	
ATOM	4482	CB	GLU	254	6.793	12.875	39.978	1.00	41.13	B	
ATOM	4483	CG	GLU	254	6.621	13.842	38.836	1.00	44.09	B	
ATOM	4484	CD	GLU	254	7.073	15.233	39.189	1.00	45.25	B	
ATOM	4485	OE1	GLU	254	6.665	15.737	40.256	1.00	45.35	B	
ATOM	4486	OE2	GLU	254	7.828	15.825	38.391	1.00	46.38	B	
ATOM	4487	C	GLU	254	6.926	10.539	40.756	1.00	39.50	B	
ATOM	4488	O	GLU	254	6.242	10.540	41.769	1.00	40.75	B	
ATOM	4489	N	LEU	255	8.008	9.779	40.614	1.00	37.82	B	
ATOM	4490	CA	LEU	255	8.484	8.894	41.676	1.00	36.11	B	
ATOM	4491	CB	LEU	255	8.895	7.543	41.087	1.00	35.93	B	
ATOM	4492	CG	LEU	255	7.950	6.910	40.062	1.00	35.67	B	
ATOM	4493	CD1	LEU	255	8.538	5.614	39.590	1.00	35.24	B	
ATOM	4494	CD2	LEU	255	6.601	6.663	40.668	1.00	35.26	B	
ATOM	4495	C	LEU	255	9.710	9.551	42.322	1.00	35.19	B	
ATOM	4496	O	LEU	255	10.722	9.754	41.644	1.00	35.09	B	

ATOM	4497	N	VAL	256	9.612	9.888	43.615	1.00	33.29	B	
ATOM	4498	CA	VAL	256	10.719	10.528	44.350	1.00	31.53	B	
ATOM	4499	CB	VAL	256	10.237	11.748	45.143	1.00	31.44	B	
ATOM	4500	CG1	VAL	256	9.719	12.800	44.188	1.00	30.73	B	
ATOM	4501	CG2	VAL	256	9.165	11.322	46.141	1.00	33.02	B	
ATOM	4502	C	VAL	256	11.494	9.622	45.319	1.00	29.50	B	
ATOM	4503	O	VAL	256	10.928	8.958	46.189	1.00	29.05	B	
ATOM	4504	N	LYS	257	12.809	9.604	45.148	1.00	27.07	B	
ATOM	4505	CA	LYS	257	13.676	8.790	45.985	1.00	24.38	B	
ATOM	4506	CB	LYS	257	14.530	7.832	45.134	1.00	21.73	B	
ATOM	4507	CG	LYS	257	13.742	6.776	44.369	1.00	18.70	B	
ATOM	4508	CD	LYS	257	14.637	5.862	43.566	1.00	13.96	B	
ATOM	4509	CE	LYS	257	15.316	6.632	42.460	1.00	12.43	B	
ATOM	4510	NZ	LYS	257	16.093	5.743	41.576	1.00	10.28	B	
ATOM	4511	C	LYS	257	14.627	9.701	46.731	1.00	23.77	B	
ATOM	4512	O	LYS	257	15.062	10.708	46.215	1.00	24.31	B	
ATOM	4513	N	ILE	258	14.928	9.357	47.970	1.00	22.97	B	
ATOM	4514	CA	ILE	258	15.882	10.138	48.741	1.00	20.65	B	
ATOM	4515	CB	ILE	258	15.226	10.866	49.913	1.00	22.22	B	
ATOM	4516	CG2	ILE	258	16.246	11.747	50.591	1.00	22.81	B	
ATOM	4517	CG1	ILE	258	14.080	11.734	49.407	1.00	24.53	B	
ATOM	4518	CD1	ILE	258	13.276	12.417	50.518	1.00	24.98	B	
ATOM	4519	C	ILE	258	16.891	9.136	49.271	1.00	18.47	B	
ATOM	4520	O	ILE	258	16.554	8.243	50.049	1.00	16.24	B	
ATOM	4521	N	GLY	259	18.123	9.256	48.805	1.00	17.79	B	
ATOM	4522	CA	GLY	259	19.144	8.342	49.262	1.00	18.70	B	
ATOM	4523	C	GLY	259	20.205	9.094	50.030	1.00	17.80	B	
ATOM	4524	O	GLY	259	20.684	10.110	49.555	1.00	18.70	B	
ATOM	4525	N	LYS	260	20.565	8.606	51.215	1.00	16.12	B	
ATOM	4526	CA	LYS	260	21.598	9.263	52.011	1.00	15.58	B	
ATOM	4527	CB	LYS	260	21.034	9.800	53.335	1.00	15.55	B	
ATOM	4528	CG	LYS	260	21.889	10.844	54.046	1.00	14.21	B	
ATOM	4529	CD	LYS	260	21.173	11.288	55.341	1.00	15.40	B	
ATOM	4530	CE	LYS	260	21.989	12.289	56.170	1.00	13.76	B	
ATOM	4531	NZ	LYS	260	21.311	12.687	57.451	1.00	8.49	B	
ATOM	4532	C	LYS	260	22.729	8.309	52.335	1.00	13.87	B	
ATOM	4533	O	LYS	260	22.531	7.185	52.741	1.00	13.84	B	
ATOM	4534	N	LEU	261	23.937	8.788	52.141	1.00	13.07	B	
ATOM	4535	CA	LEU	261	25.107	7.996	52.430	1.00	11.82	B	
ATOM	4536	CB	LEU	261	25.890	7.772	51.130	1.00	10.77	B	
ATOM	4537	CG	LEU	261	27.276	7.138	51.238	1.00	8.89	B	
ATOM	4538	CD1	LEU	261	27.189	5.799	51.975	1.00	7.84	B	
ATOM	4539	CD2	LEU	261	27.847	6.973	49.840	1.00	7.48	B	
ATOM	4540	C	LEU	261	25.993	8.696	53.465	1.00	11.44	B	
ATOM	4541	O	LEU	261	26.424	9.819	53.247	1.00	13.74	B	
ATOM	4542	N	ASN	262	26.245	8.024	54.586	1.00	10.57	B	
ATOM	4543	CA	ASN	262	27.142	8.548	55.615	1.00	8.04	B	
ATOM	4544	CB	ASN	262	26.494	8.386	56.985	1.00	5.60	B	
ATOM	4545	CG	ASN	262	25.111	8.980	57.011	1.00	8.99	B	
ATOM	4546	OD1	ASN	262	24.100	8.263	56.971	1.00	9.21	B	
ATOM	4547	ND2	ASN	262	25.050	10.307	57.024	1.00	7.62	B	
ATOM	4548	C	ASN	262	28.526	7.879	55.554	1.00	6.87	B	
ATOM	4549	O	ASN	262	28.640	6.653	55.523	1.00	7.74	B	
ATOM	4550	N	LEU	263	29.566	8.705	55.487	1.00	5.79	B	
ATOM	4551	CA	LEU	263	30.938	8.225	55.438	1.00	5.65	B	
ATOM	4552	CB	LEU	263	31.596	8.741	54.165	1.00	4.90	B	
ATOM	4553	CG	LEU	263	30.735	8.279	52.998	1.00	6.08	B	
ATOM	4554	CD1	LEU	263	31.131	9.012	51.752	1.00	5.33	B	
ATOM	4555	CD2	LEU	263	30.853	6.748	52.877	1.00	6.04	B	
ATOM	4556	C	LEU	263	31.634	8.694	56.710	1.00	6.26	B	
ATOM	4557	O	LEU	263	32.017	9.853	56.842	1.00	8.01	B	
ATOM	4558	N	VAL	264	31.795	7.778	57.653	1.00	6.21	B	
ATOM	4559	CA	VAL	264	32.406	8.079	58.943	1.00	6.25	B	
ATOM	4560	CB	VAL	264	31.600	7.410	60.037	1.00	7.30	B	
ATOM	4561	CG1	VAL	264	32.081	7.848	61.406	1.00	6.21	B	
ATOM	4562	CG2	VAL	264	30.140	7.709	59.802	1.00	9.51	B	
ATOM	4563	C	VAL	264	33.863	7.677	59.150	1.00	7.28	B	
ATOM	4564	O	VAL	264	34.221	6.532	58.978	1.00	7.31	B	
ATOM	4565	N	ASP	265	34.685	8.652	59.533	1.00	9.79	B	
ATOM	4566	CA	ASP	265	36.105	8.441	59.841	1.00	11.34	B	
ATOM	4567	CB	ASP	265	36.978	9.564	59.262	1.00	12.62	B	
ATOM	4568	CG	ASP	265	38.473	9.346	59.520	1.00	16.17	B	
ATOM	4569	OD1	ASP	265	38.801	8.748	60.562	1.00	17.08	B	

ATOM	4570	OD2	ASP	265	39.310	9.783	58.694	1.00	16.43	B
ATOM	4571	C	ASP	265	36.179	8.527	61.374	1.00	11.75	B
ATOM	4572	O	ASP	265	36.356	9.601	61.928	1.00	11.74	B
ATOM	4573	N	LEU	266	36.032	7.389	62.051	1.00	12.21	B
ATOM	4574	CA	LEU	266	36.054	7.367	63.519	1.00	13.54	B
ATOM	4575	CB	LEU	266	35.692	5.986	64.068	1.00	13.06	B
ATOM	4576	CG	LEU	266	34.327	5.426	63.711	1.00	14.69	B
ATOM	4577	CD1	LEU	266	34.190	3.979	64.232	1.00	13.37	B
ATOM	4578	CD2	LEU	266	33.266	6.350	64.285	1.00	14.29	B
ATOM	4579	C	LEU	266	37.366	7.763	64.193	1.00	14.66	B
ATOM	4580	O	LEU	266	38.437	7.776	63.580	1.00	16.77	B
ATOM	4581	N	ALA	267	37.267	8.097	65.474	1.00	15.57	B
ATOM	4582	CA	ALA	267	38.435	8.494	66.237	1.00	15.49	B
ATOM	4583	CB	ALA	267	38.015	9.063	67.584	1.00	15.66	B
ATOM	4584	C	ALA	267	39.281	7.256	66.427	1.00	16.90	B
ATOM	4585	O	ALA	267	38.752	6.166	66.492	1.00	17.09	B
ATOM	4586	N	GLY	268	40.594	7.432	66.535	1.00	18.45	B
ATOM	4587	CA	GLY	268	41.470	6.286	66.684	1.00	19.06	B
ATOM	4588	C	GLY	268	40.979	5.375	67.779	1.00	20.29	B
ATOM	4589	O	GLY	268	40.476	5.846	68.778	1.00	22.63	B
ATOM	4590	N	SER	269	41.153	4.070	67.608	1.00	21.30	B
ATOM	4591	CA	SER	269	40.683	3.127	68.611	1.00	21.55	B
ATOM	4592	CB	SER	269	40.151	1.869	67.940	1.00	19.85	B
ATOM	4593	OG	SER	269	41.174	1.230	67.206	1.00	19.77	B
ATOM	4594	C	SER	269	41.696	2.703	69.666	1.00	23.07	B
ATOM	4595	O	SER	269	41.415	1.832	70.461	1.00	23.77	B
ATOM	4596	N	GLU	270	42.863	3.336	69.682	1.00	24.72	B
ATOM	4597	CA	GLU	270	43.889	2.997	70.666	1.00	26.45	B
ATOM	4598	CB	GLU	270	45.255	3.538	70.212	1.00	26.88	B
ATOM	4599	CG	GLU	270	45.365	5.074	70.179	1.00	26.65	B
ATOM	4600	CD	GLU	270	44.769	5.716	68.938	1.00	25.63	B
ATOM	4601	OE1	GLU	270	44.782	6.966	68.848	1.00	25.90	B
ATOM	4602	OE2	GLU	270	44.299	4.966	68.063	1.00	25.37	B
ATOM	4603	C	GLU	270	43.595	3.501	72.096	1.00	28.21	B
ATOM	4604	O	GLU	270	43.182	4.646	72.317	1.00	27.82	B
ATOM	4605	N	ASN	271	43.804	2.619	73.066	1.00	31.11	B
ATOM	4606	CA	ASN	271	43.590	2.932	74.483	1.00	33.53	B
ATOM	4607	CB	ASN	271	42.239	3.620	74.720	1.00	35.28	B
ATOM	4608	CG	ASN	271	41.046	2.755	74.319	1.00	37.15	B
ATOM	4609	OD1	ASN	271	39.892	3.159	74.481	1.00	37.89	B
ATOM	4610	ND2	ASN	271	41.319	1.569	73.789	1.00	38.13	B
ATOM	4611	C	ASN	271	43.617	1.669	75.326	1.00	34.61	B
ATOM	4612	O	ASN	271	43.637	0.561	74.789	1.00	35.03	B
ATOM	4613	N	ASN	287	41.713	11.898	79.742	1.00	41.72	B
ATOM	4614	CA	ASN	287	40.726	12.291	78.737	1.00	42.10	B
ATOM	4615	CB	ASN	287	41.389	13.166	77.666	1.00	43.36	B
ATOM	4616	CG	ASN	287	42.137	14.334	78.263	1.00	44.01	B
ATOM	4617	OD1	ASN	287	43.107	14.144	78.990	1.00	44.40	B
ATOM	4618	ND2	ASN	287	41.688	15.548	77.967	1.00	44.56	B
ATOM	4619	C	ASN	287	40.094	11.054	78.083	1.00	41.01	B
ATOM	4620	O	ASN	287	40.802	10.130	77.661	1.00	42.34	B
ATOM	4621	N	ILE	288	38.764	11.039	77.994	1.00	37.53	B
ATOM	4622	CA	ILE	288	38.053	9.905	77.397	1.00	33.20	B
ATOM	4623	CB	ILE	288	37.119	9.256	78.433	1.00	33.55	B
ATOM	4624	CG2	ILE	288	37.940	8.681	79.575	1.00	32.67	B
ATOM	4625	CG1	ILE	288	36.142	10.308	78.967	1.00	33.79	B
ATOM	4626	CD1	ILE	288	35.028	9.764	79.828	1.00	33.58	B
ATOM	4627	C	ILE	288	37.221	10.255	76.147	1.00	29.09	B
ATOM	4628	O	ILE	288	36.810	11.410	75.946	1.00	28.30	B
ATOM	4629	N	ASN	289	36.975	9.258	75.303	1.00	23.27	B
ATOM	4630	CA	ASN	289	36.172	9.492	74.116	1.00	19.88	B
ATOM	4631	CB	ASN	289	36.898	8.993	72.871	1.00	18.84	B
ATOM	4632	CG	ASN	289	36.379	9.622	71.601	1.00	19.35	B
ATOM	4633	OD1	ASN	289	37.155	10.094	70.786	1.00	21.16	B
ATOM	4634	ND2	ASN	289	35.065	9.612	71.415	1.00	18.98	B
ATOM	4635	C	ASN	289	34.829	8.805	74.326	1.00	18.28	B
ATOM	4636	O	ASN	289	34.628	7.609	74.013	1.00	16.89	B
ATOM	4637	N	GLN	290	33.906	9.579	74.884	1.00	16.97	B
ATOM	4638	CA	GLN	290	32.560	9.115	75.178	1.00	14.08	B
ATOM	4639	CB	GLN	290	31.741	10.277	75.738	1.00	15.20	B
ATOM	4640	CG	GLN	290	30.328	9.905	76.161	1.00	16.32	B
ATOM	4641	CD	GLN	290	30.274	8.855	77.266	1.00	16.30	B
ATOM	4642	OE1	GLN	290	29.232	8.273	77.512	1.00	16.57	B

ATOM	4643	NE2	GLN	290	31.401	8.621	77.934	1.00	17.40	B
ATOM	4644	C	GLN	290	31.856	8.520	73.959	1.00	12.46	B
ATOM	4645	O	GLN	290	31.207	7.500	74.055	1.00	12.26	B
ATOM	4646	N	SER	291	31.971	9.174	72.814	1.00	11.04	B
ATOM	4647	CA	SER	291	31.333	8.627	71.629	1.00	11.96	B
ATOM	4648	CB	SER	291	31.404	9.609	70.466	1.00	11.35	B
ATOM	4649	OG	SER	291	30.393	10.586	70.582	1.00	12.37	B
ATOM	4650	C	SER	291	31.950	7.299	71.201	1.00	11.18	B
ATOM	4651	O	SER	291	31.241	6.375	70.783	1.00	11.32	B
ATOM	4652	N	LEU	292	33.270	7.205	71.294	1.00	11.69	B
ATOM	4653	CA	LEU	292	33.965	5.984	70.919	1.00	11.36	B
ATOM	4654	CB	LEU	292	35.485	6.237	70.902	1.00	9.67	B
ATOM	4655	CG	LEU	292	36.263	5.054	70.334	1.00	10.97	B
ATOM	4656	CD1	LEU	292	35.817	4.822	68.911	1.00	10.21	B
ATOM	4657	CD2	LEU	292	37.750	5.328	70.387	1.00	13.35	B
ATOM	4658	C	LEU	292	33.574	4.877	71.914	1.00	11.82	B
ATOM	4659	O	LEU	292	33.287	3.724	71.527	1.00	11.11	B
ATOM	4660	N	LEU	293	33.547	5.232	73.194	1.00	8.02	B
ATOM	4661	CA	LEU	293	33.210	4.295	74.246	1.00	7.35	B
ATOM	4662	CB	LEU	293	33.313	5.005	75.596	1.00	5.38	B
ATOM	4663	CG	LEU	293	34.410	4.587	76.570	1.00	6.04	B
ATOM	4664	CD1	LEU	293	35.605	3.981	75.841	1.00	3.22	B
ATOM	4665	CD2	LEU	293	34.798	5.808	77.389	1.00	3.25	B
ATOM	4666	C	LEU	293	31.802	3.747	74.071	1.00	7.33	B
ATOM	4667	O	LEU	293	31.563	2.550	74.222	1.00	9.04	B
ATOM	4668	N	THR	294	30.874	4.646	73.775	1.00	8.36	B
ATOM	4669	CA	THR	294	29.481	4.283	73.604	1.00	6.48	B
ATOM	4670	CB	THR	294	28.623	5.535	73.600	1.00	5.81	B
ATOM	4671	OG1	THR	294	28.889	6.251	74.804	1.00	6.32	B
ATOM	4672	CG2	THR	294	27.142	5.206	73.570	1.00	4.45	B
ATOM	4673	C	THR	294	29.237	3.461	72.364	1.00	7.94	B
ATOM	4674	O	THR	294	28.357	2.602	72.368	1.00	9.76	B
ATOM	4675	N	LEU	295	30.016	3.706	71.310	1.00	6.67	B
ATOM	4676	CA	LEU	295	29.896	2.918	70.074	1.00	6.68	B
ATOM	4677	CB	LEU	295	30.931	3.313	69.016	1.00	6.59	B
ATOM	4678	CG	LEU	295	30.897	2.510	67.708	1.00	5.44	B
ATOM	4679	CD1	LEU	295	29.555	2.668	67.036	1.00	4.15	B
ATOM	4680	CD2	LEU	295	31.969	2.993	66.786	1.00	5.26	B
ATOM	4681	C	LEU	295	30.228	1.473	70.403	1.00	8.24	B
ATOM	4682	O	LEU	295	29.615	0.555	69.887	1.00	9.80	B
ATOM	4683	N	GLY	296	31.214	1.290	71.276	1.00	9.60	B
ATOM	4684	CA	GLY	296	31.611	-0.047	71.669	1.00	10.99	B
ATOM	4685	C	GLY	296	30.551	-0.728	72.518	1.00	12.56	B
ATOM	4686	O	GLY	296	30.275	-1.924	72.350	1.00	12.84	B
ATOM	4687	N	ARG	297	29.954	0.037	73.426	1.00	12.22	B
ATOM	4688	CA	ARG	297	28.928	-0.486	74.307	1.00	12.41	B
ATOM	4689	CB	ARG	297	28.692	0.466	75.478	1.00	11.73	B
ATOM	4690	CG	ARG	297	29.818	0.493	76.498	1.00	10.69	B
ATOM	4691	CD	ARG	297	29.767	1.736	77.378	1.00	11.84	B
ATOM	4692	NE	ARG	297	30.969	1.856	78.205	1.00	10.74	B
ATOM	4693	CZ	ARG	297	31.409	2.993	78.734	1.00	10.49	B
ATOM	4694	NH1	ARG	297	30.743	4.119	78.517	1.00	11.64	B
ATOM	4695	NH2	ARG	297	32.504	3.003	79.486	1.00	9.73	B
ATOM	4696	C	ARG	297	27.622	-0.708	73.569	1.00	13.86	B
ATOM	4697	O	ARG	297	26.798	-1.514	74.009	1.00	13.06	B
ATOM	4698	N	VAL	298	27.426	0.014	72.464	1.00	14.33	B
ATOM	4699	CA	VAL	298	26.216	-0.134	71.659	1.00	16.21	B
ATOM	4700	CB	VAL	298	26.048	1.031	70.696	1.00	16.05	B
ATOM	4701	CG1	VAL	298	25.021	0.679	69.639	1.00	17.88	B
ATOM	4702	CG2	VAL	298	25.605	2.257	71.458	1.00	18.13	B
ATOM	4703	C	VAL	298	26.281	-1.426	70.853	1.00	17.16	B
ATOM	4704	O	VAL	298	25.305	-2.173	70.774	1.00	18.74	B
ATOM	4705	N	ILE	299	27.441	-1.691	70.262	1.00	18.24	B
ATOM	4706	CA	ILE	299	27.645	-2.910	69.486	1.00	18.96	B
ATOM	4707	CB	ILE	299	29.019	-2.868	68.770	1.00	19.68	B
ATOM	4708	CG2	ILE	299	29.368	-4.245	68.184	1.00	17.64	B
ATOM	4709	CG1	ILE	299	28.983	-1.791	67.674	1.00	19.70	B
ATOM	4710	CD1	ILE	299	30.314	-1.589	66.977	1.00	22.74	B
ATOM	4711	C	ILE	299	27.551	-4.142	70.400	1.00	19.56	B
ATOM	4712	O	ILE	299	27.027	-5.191	70.012	1.00	19.03	B
ATOM	4713	N	THR	300	28.043	-4.017	71.624	1.00	19.86	B
ATOM	4714	CA	THR	300	27.978	-5.136	72.551	1.00	20.92	B
ATOM	4715	CB	THR	300	28.770	-4.841	73.824	1.00	20.58	B

ATOM	4716	OG1	THR	300	30.172	-4.893	73.533	1.00	21.97	B
ATOM	4717	CG2	THR	300	28.433	-5.845	74.903	1.00	21.65	B
ATOM	4718	C	THR	300	26.525	-5.450	72.915	1.00	21.71	B
ATOM	4719	O	THR	300	26.134	-6.601	72.984	1.00	22.71	B
ATOM	4720	N	ALA	301	25.728	-4.413	73.139	1.00	23.13	B
ATOM	4721	CA	ALA	301	24.337	-4.624	73.494	1.00	23.01	B
ATOM	4722	CB	ALA	301	23.694	-3.327	73.904	1.00	22.73	B
ATOM	4723	C	ALA	301	23.589	-5.225	72.323	1.00	23.48	B
ATOM	4724	O	ALA	301	22.652	-5.982	72.509	1.00	23.63	B
ATOM	4725	N	LEU	302	24.005	-4.872	71.111	1.00	23.21	B
ATOM	4726	CA	LEU	302	23.361	-5.392	69.911	1.00	24.59	B
ATOM	4727	CB	LEU	302	23.737	-4.526	68.695	1.00	23.93	B
ATOM	4728	CG	LEU	302	22.774	-3.511	68.059	1.00	22.99	B
ATOM	4729	CD1	LEU	302	21.827	-2.952	69.058	1.00	20.71	B
ATOM	4730	CD2	LEU	302	23.579	-2.394	67.440	1.00	21.49	B
ATOM	4731	C	LEU	302	23.728	-6.861	69.656	1.00	25.70	B
ATOM	4732	O	LEU	302	22.847	-7.695	69.406	1.00	24.83	B
ATOM	4733	N	VAL	303	25.021	-7.170	69.731	1.00	27.74	B
ATOM	4734	CA	VAL	303	25.527	-8.521	69.505	1.00	29.35	B
ATOM	4735	CB	VAL	303	27.054	-8.549	69.593	1.00	29.55	B
ATOM	4736	CG1	VAL	303	27.545	-9.975	69.439	1.00	30.49	B
ATOM	4737	CG2	VAL	303	27.651	-7.641	68.524	1.00	30.24	B
ATOM	4738	C	VAL	303	24.985	-9.528	70.510	1.00	31.00	B
ATOM	4739	O	VAL	303	24.629	-10.631	70.160	1.00	30.43	B
ATOM	4740	N	GLU	304	24.927	-9.123	71.770	1.00	33.86	B
ATOM	4741	CA	GLU	304	24.442	-9.986	72.838	1.00	36.40	B
ATOM	4742	CB	GLU	304	25.130	-9.594	74.143	1.00	37.33	B
ATOM	4743	CG	GLU	304	26.650	-9.690	74.076	1.00	39.18	B
ATOM	4744	CD	GLU	304	27.316	-9.437	75.422	1.00	41.19	B
ATOM	4745	OE1	GLU	304	28.564	-9.473	75.490	1.00	42.27	B
ATOM	4746	OE2	GLU	304	26.594	-9.202	76.413	1.00	42.10	B
ATOM	4747	C	GLU	304	22.922	-9.924	72.985	1.00	38.11	B
ATOM	4748	O	GLU	304	22.334	-10.552	73.871	1.00	37.60	B
ATOM	4749	N	ARG	305	22.303	-9.155	72.098	1.00	41.03	B
ATOM	4750	CA	ARG	305	20.860	-8.996	72.068	1.00	43.26	B
ATOM	4751	CB	ARG	305	20.221	-10.302	71.592	1.00	44.67	B
ATOM	4752	CG	ARG	305	20.602	-10.629	70.151	1.00	46.86	B
ATOM	4753	CD	ARG	305	20.167	-12.025	69.716	1.00	49.68	B
ATOM	4754	NE	ARG	305	20.654	-12.350	68.373	1.00	50.79	B
ATOM	4755	CZ	ARG	305	20.244	-11.753	67.258	1.00	50.97	B
ATOM	4756	NH1	ARG	305	19.327	-10.797	67.309	1.00	51.47	B
ATOM	4757	NH2	ARG	305	20.769	-12.097	66.089	1.00	51.54	B
ATOM	4758	C	ARG	305	20.237	-8.514	73.367	1.00	43.49	B
ATOM	4759	O	ARG	305	19.142	-8.909	73.718	1.00	44.11	B
ATOM	4760	N	THR	306	20.951	-7.648	74.077	1.00	44.17	B
ATOM	4761	CA	THR	306	20.444	-7.078	75.319	1.00	43.76	B
ATOM	4762	CB	THR	306	21.535	-6.267	76.040	1.00	43.72	B
ATOM	4763	OG1	THR	306	22.623	-7.131	76.399	1.00	43.84	B
ATOM	4764	CG2	THR	306	20.975	-5.602	77.288	1.00	43.30	B
ATOM	4765	C	THR	306	19.307	-6.139	74.912	1.00	44.17	B
ATOM	4766	O	THR	306	19.388	-5.459	73.891	1.00	45.09	B
ATOM	4767	N	PRO	307	18.226	-6.098	75.700	1.00	43.54	B
ATOM	4768	CD	PRO	307	17.925	-6.973	76.846	1.00	43.66	B
ATOM	4769	CA	PRO	307	17.080	-5.232	75.390	1.00	42.75	B
ATOM	4770	CB	PRO	307	16.101	-5.554	76.518	1.00	43.35	B
ATOM	4771	CG	PRO	307	16.429	-7.001	76.834	1.00	44.16	B
ATOM	4772	C	PRO	307	17.408	-3.741	75.269	1.00	41.65	B
ATOM	4773	O	PRO	307	16.903	-3.049	74.384	1.00	41.15	B
ATOM	4774	N	HIS	308	18.254	-3.247	76.166	1.00	39.72	B
ATOM	4775	CA	HIS	308	18.629	-1.839	76.164	1.00	37.51	B
ATOM	4776	CB	HIS	308	18.774	-1.336	77.587	1.00	39.81	B
ATOM	4777	CG	HIS	308	19.193	0.097	77.677	1.00	42.26	B
ATOM	4778	CD2	HIS	308	20.336	0.664	78.127	1.00	43.26	B
ATOM	4779	ND1	HIS	308	18.391	1.131	77.247	1.00	43.54	B
ATOM	4780	CE1	HIS	308	19.024	2.278	77.428	1.00	44.49	B
ATOM	4781	NE2	HIS	308	20.205	2.024	77.959	1.00	44.29	B
ATOM	4782	C	HIS	308	19.937	-1.559	75.446	1.00	35.63	B
ATOM	4783	O	HIS	308	20.958	-2.160	75.745	1.00	36.69	B
ATOM	4784	N	VAL	309	19.889	-0.627	74.501	1.00	32.04	B
ATOM	4785	CA	VAL	309	21.071	-0.237	73.731	1.00	27.44	B
ATOM	4786	CB	VAL	309	20.821	-0.415	72.218	1.00	27.23	B
ATOM	4787	CG1	VAL	309	22.090	-0.111	71.426	1.00	27.83	B
ATOM	4788	CG2	VAL	309	20.336	-1.823	71.946	1.00	25.00	B

ATOM	4789	C	VAL	309	21.307	1.234	74.059	1.00	26.45	B	
ATOM	4790	O	VAL	309	20.501	2.090	73.724	1.00	26.41	B	
ATOM	4791	N	PRO	310	22.432	1.538	74.715	1.00	25.12	B	
ATOM	4792	CD	PRO	310	23.508	0.587	75.062	1.00	23.57	B	
ATOM	4793	CA	PRO	310	22.780	2.914	75.107	1.00	22.73	B	
ATOM	4794	CB	PRO	310	23.985	2.701	76.007	1.00	23.56	B	
ATOM	4795	CG	PRO	310	24.671	1.504	75.354	1.00	23.96	B	
ATOM	4796	C	PRO	310	23.017	3.958	73.999	1.00	22.22	B	
ATOM	4797	O	PRO	310	23.965	4.735	74.073	1.00	21.14	B	
ATOM	4798	N	TYR	311	22.147	4.000	72.995	1.00	21.70	B	
ATOM	4799	CA	TYR	311	22.294	4.967	71.899	1.00	22.33	B	
ATOM	4800	CB	TYR	311	21.083	4.978	70.970	1.00	22.30	B	
ATOM	4801	CG	TYR	311	20.861	3.721	70.154	1.00	24.68	B	
ATOM	4802	CD1	TYR	311	21.773	3.322	69.177	1.00	25.08	B	
ATOM	4803	CE1	TYR	311	21.555	2.171	68.411	1.00	25.18	B	
ATOM	4804	CD2	TYR	311	19.717	2.937	70.347	1.00	24.09	B	
ATOM	4805	CE2	TYR	311	19.493	1.786	69.590	1.00	24.09	B	
ATOM	4806	CZ	TYR	311	20.416	1.405	68.623	1.00	24.98	B	
ATOM	4807	OH	TYR	311	20.211	0.246	67.893	1.00	24.66	B	
ATOM	4808	C	TYR	311	22.431	6.429	72.338	1.00	21.98	B	
ATOM	4809	O	TYR	311	23.180	7.188	71.741	1.00	23.57	B	
ATOM	4810	N	ARG	312	21.707	6.813	73.384	1.00	20.49	B	
ATOM	4811	CA	ARG	312	21.726	8.203	73.861	1.00	19.38	B	
ATOM	4812	CB	ARG	312	20.447	8.544	74.640	1.00	21.56	B	
ATOM	4813	CG	ARG	312	19.150	8.149	73.951	1.00	24.98	B	
ATOM	4814	CD	ARG	312	17.949	8.887	74.534	1.00	27.94	B	
ATOM	4815	NE	ARG	312	16.688	8.240	74.175	1.00	31.63	B	
ATOM	4816	CZ	ARG	312	16.262	7.086	74.688	1.00	34.10	B	
ATOM	4817	NH1	ARG	312	16.996	6.445	75.590	1.00	37.15	B	
ATOM	4818	NH2	ARG	312	15.101	6.566	74.304	1.00	33.60	B	
ATOM	4819	C	ARG	312	22.875	8.612	74.779	1.00	17.27	B	
ATOM	4820	O	ARG	312	22.933	9.756	75.235	1.00	16.64	B	
ATOM	4821	N	GLU	313	23.786	7.686	75.054	1.00	14.25	B	
ATOM	4822	CA	GLU	313	24.908	7.986	75.935	1.00	11.55	B	
ATOM	4823	CB	GLU	313	25.410	6.693	76.590	1.00	11.14	B	
ATOM	4824	CG	GLU	313	24.416	6.136	77.618	1.00	11.41	B	
ATOM	4825	CD	GLU	313	24.916	4.905	78.379	1.00	12.57	B	
ATOM	4826	OE1	GLU	313	26.071	4.898	78.834	1.00	11.41	B	
ATOM	4827	OE2	GLU	313	24.149	3.935	78.569	1.00	14.80	B	
ATOM	4828	C	GLU	313	26.053	8.746	75.271	1.00	10.23	B	
ATOM	4829	O	GLU	313	27.066	8.960	75.891	1.00	10.15	B	
ATOM	4830	N	SER	314	25.865	9.164	74.017	1.00	10.36	B	
ATOM	4831	CA	SER	314	26.878	9.912	73.263	1.00	9.41	B	
ATOM	4832	CB	SER	314	28.000	9.018	72.732	1.00	10.81	B	
ATOM	4833	OG	SER	314	27.643	8.320	71.544	1.00	9.64	B	
ATOM	4834	C	SER	314	26.235	10.511	72.031	1.00	10.05	B	
ATOM	4835	O	SER	314	25.190	10.052	71.583	1.00	9.18	B	
ATOM	4836	N	LYS	315	26.887	11.544	71.501	1.00	10.81	B	
ATOM	4837	CA	LYS	315	26.428	12.259	70.320	1.00	9.07	B	
ATOM	4838	CB	LYS	315	27.254	13.527	70.063	1.00	9.50	B	
ATOM	4839	CG	LYS	315	27.390	14.463	71.236	1.00	9.25	B	
ATOM	4840	CD	LYS	315	26.058	14.973	71.686	1.00	10.89	B	
ATOM	4841	CE	LYS	315	26.244	16.156	72.620	1.00	13.02	B	
ATOM	4842	NZ	LYS	315	26.918	17.316	71.937	1.00	14.10	B	
ATOM	4843	C	LYS	315	26.556	11.414	69.077	1.00	8.68	B	
ATOM	4844	O	LYS	315	25.652	11.383	68.282	1.00	10.14	B	
ATOM	4845	N	LEU	316	27.683	10.721	68.931	1.00	8.28	B	
ATOM	4846	CA	LEU	316	27.928	9.888	67.763	1.00	7.48	B	
ATOM	4847	CB	LEU	316	29.297	9.205	67.867	1.00	6.90	B	
ATOM	4848	CG	LEU	316	29.679	8.277	66.713	1.00	8.06	B	
ATOM	4849	CD1	LEU	316	30.018	9.097	65.484	1.00	10.24	B	
ATOM	4850	CD2	LEU	316	30.850	7.452	67.129	1.00	8.22	B	
ATOM	4851	C	LEU	316	26.852	8.821	67.590	1.00	9.38	B	
ATOM	4852	O	LEU	316	26.241	8.733	66.523	1.00	9.82	B	
ATOM	4853	N	THR	317	26.588	8.040	68.642	1.00	9.80	B	
ATOM	4854	CA	THR	317	25.599	6.965	68.534	1.00	10.18	B	
ATOM	4855	CB	THR	317	25.672	5.952	69.674	1.00	10.15	B	
ATOM	4856	OG1	THR	317	25.527	6.642	70.909	1.00	10.81	B	
ATOM	4857	CG2	THR	317	27.004	5.185	69.661	1.00	9.59	B	
ATOM	4858	C	THR	317	24.175	7.455	68.484	1.00	10.03	B	
ATOM	4859	O	THR	317	23.295	6.709	68.146	1.00	11.71	B	
ATOM	4860	N	ARG	318	23.947	8.703	68.867	1.00	9.69	B	
ATOM	4861	CA	ARG	318	22.607	9.256	68.785	1.00	9.04	B	

ATOM	4862	CB	ARG	318	22.454	10.464	69.703	1.00	13.23	B	
ATOM	4863	CG	ARG	318	21.719	10.147	71.004	1.00	19.08	B	
ATOM	4864	CD	ARG	318	22.058	11.133	72.115	1.00	22.73	B	
ATOM	4865	NE	ARG	318	21.617	12.495	71.828	1.00	26.31	B	
ATOM	4866	CZ	ARG	318	20.345	12.863	71.705	1.00	27.29	B	
ATOM	4867	NH1	ARG	318	19.383	11.963	71.849	1.00	28.67	B	
ATOM	4868	NH2	ARG	318	20.036	14.124	71.429	1.00	25.94	B	
ATOM	4869	C	ARG	318	22.434	9.679	67.344	1.00	8.51	B	
ATOM	4870	O	ARG	318	21.418	9.412	66.720	1.00	10.84	B	
ATOM	4871	N	ILE	319	23.445	10.339	66.799	1.00	5.66	B	
ATOM	4872	CA	ILE	319	23.352	10.766	65.410	1.00	5.05	B	
ATOM	4873	CB	ILE	319	24.591	11.627	65.014	1.00	5.19	B	
ATOM	4874	CG2	ILE	319	24.531	11.976	63.544	1.00	6.51	B	
ATOM	4875	CG1	ILE	319	24.603	12.935	65.826	1.00	5.47	B	
ATOM	4876	CD1	ILE	319	25.833	13.774	65.632	1.00	2.71	B	
ATOM	4877	C	ILE	319	23.227	9.551	64.460	1.00	3.03	B	
ATOM	4878	O	ILE	319	22.361	9.511	63.590	1.00	1.95	B	
ATOM	4879	N	LEU	320	24.067	8.540	64.657	1.00	4.41	B	
ATOM	4880	CA	LEU	320	24.056	7.376	63.767	1.00	5.60	B	
ATOM	4881	CB	LEU	320	25.490	6.931	63.451	1.00	2.81	B	
ATOM	4882	CG	LEU	320	26.437	7.964	62.845	1.00	2.57	B	
ATOM	4883	CD1	LEU	320	27.873	7.442	62.786	1.00	2.20	B	
ATOM	4884	CD2	LEU	320	25.955	8.334	61.476	1.00	1.00	B	
ATOM	4885	C	LEU	320	23.313	6.122	64.235	1.00	7.52	B	
ATOM	4886	O	LEU	320	23.620	5.045	63.776	1.00	7.94	B	
ATOM	4887	N	GLN	321	22.306	6.258	65.094	1.00	10.60	B	
ATOM	4888	CA	GLN	321	21.629	5.057	65.604	1.00	16.44	B	
ATOM	4889	CB	GLN	321	20.679	5.362	66.775	1.00	18.94	B	
ATOM	4890	CG	GLN	321	19.433	6.153	66.458	1.00	22.43	B	
ATOM	4891	CD	GLN	321	18.593	6.391	67.707	1.00	25.16	B	
ATOM	4892	OE1	GLN	321	18.121	5.453	68.338	1.00	26.09	B	
ATOM	4893	NE2	GLN	321	18.418	7.658	68.071	1.00	26.05	B	
ATOM	4894	C	GLN	321	20.882	4.186	64.617	1.00	16.64	B	
ATOM	4895	O	GLN	321	20.700	2.992	64.870	1.00	16.23	B	
ATOM	4896	N	ASP	322	20.439	4.759	63.505	1.00	17.01	B	
ATOM	4897	CA	ASP	322	19.762	3.931	62.521	1.00	19.03	B	
ATOM	4898	CB	ASP	322	18.952	4.755	61.535	1.00	20.75	B	
ATOM	4899	CG	ASP	322	17.983	3.896	60.727	1.00	22.50	B	
ATOM	4900	OD1	ASP	322	17.835	4.125	59.506	1.00	24.17	B	
ATOM	4901	OD2	ASP	322	17.352	2.997	61.327	1.00	21.00	B	
ATOM	4902	C	ASP	322	20.803	3.139	61.722	1.00	20.46	B	
ATOM	4903	O	ASP	322	20.467	2.335	60.861	1.00	23.04	B	
ATOM	4904	N	SER	323	22.076	3.385	62.006	1.00	20.16	B	
ATOM	4905	CA	SER	323	23.164	2.670	61.353	1.00	18.88	B	
ATOM	4906	CB	SER	323	24.299	3.643	61.077	1.00	17.96	B	
ATOM	4907	OG	SER	323	23.842	4.642	60.187	1.00	18.62	B	
ATOM	4908	C	SER	323	23.625	1.518	62.259	1.00	18.52	B	
ATOM	4909	O	SER	323	24.368	0.647	61.838	1.00	19.83	B	
ATOM	4910	N	LEU	324	23.168	1.512	63.507	1.00	16.09	B	
ATOM	4911	CA	LEU	324	23.541	0.449	64.420	1.00	16.61	B	
ATOM	4912	CB	LEU	324	24.257	1.026	65.648	1.00	15.87	B	
ATOM	4913	CG	LEU	324	25.679	1.595	65.539	1.00	14.59	B	
ATOM	4914	CD1	LEU	324	26.545	0.643	64.722	1.00	13.37	B	
ATOM	4915	CD2	LEU	324	25.649	2.965	64.909	1.00	11.67	B	
ATOM	4916	C	LEU	324	22.300	-0.343	64.834	1.00	17.48	B	
ATOM	4917	O	LEU	324	21.651	-0.025	65.814	1.00	16.83	B	
ATOM	4918	N	GLY	325	21.983	-1.387	64.071	1.00	17.97	B	
ATOM	4919	CA	GLY	325	20.818	-2.203	64.377	1.00	18.49	B	
ATOM	4920	C	GLY	325	19.498	-1.576	63.939	1.00	19.29	B	
ATOM	4921	O	GLY	325	18.427	-1.950	64.423	1.00	19.24	B	
ATOM	4922	N	GLY	326	19.573	-0.630	63.007	1.00	19.01	B	
ATOM	4923	CA	GLY	326	18.382	0.052	62.539	1.00	18.79	B	
ATOM	4924	C	GLY	326	17.935	-0.373	61.165	1.00	19.04	B	
ATOM	4925	O	GLY	326	17.931	-1.550	60.861	1.00	18.81	B	
ATOM	4926	N	ARG	327	17.565	0.603	60.341	1.00	19.26	B	
ATOM	4927	CA	ARG	327	17.106	0.336	58.991	1.00	20.71	B	
ATOM	4928	CB	ARG	327	15.731	0.970	58.761	1.00	22.28	B	
ATOM	4929	CG	ARG	327	14.591	0.225	59.443	1.00	25.87	B	
ATOM	4930	CD	ARG	327	13.233	0.703	58.976	1.00	28.38	B	
ATOM	4931	NE	ARG	327	12.260	-0.388	58.957	1.00	33.27	B	
ATOM	4932	CZ	ARG	327	12.370	-1.477	58.193	1.00	36.86	B	
ATOM	4933	NH1	ARG	327	13.412	-1.639	57.382	1.00	38.23	B	
ATOM	4934	NH2	ARG	327	11.422	-2.399	58.213	1.00	38.97	B	

ATOM	4935	C	ARG	327	18.072	0.784	57.899	1.00	20.64	B	
ATOM	4936	O	ARG	327	17.721	0.788	56.718	1.00	19.55	B	
ATOM	4937	N	THR	328	19.295	1.127	58.293	1.00	19.88	B	
ATOM	4938	CA	THR	328	20.316	1.568	57.349	1.00	18.38	B	
ATOM	4939	CB	THR	328	21.133	2.694	57.948	1.00	16.59	B	
ATOM	4940	OG1	THR	328	20.260	3.780	58.254	1.00	15.01	B	
ATOM	4941	CG2	THR	328	22.170	3.171	56.975	1.00	16.39	B	
ATOM	4942	C	THR	328	21.271	0.449	56.971	1.00	17.88	B	
ATOM	4943	O	THR	328	21.640	-0.343	57.808	1.00	18.85	B	
ATOM	4944	N	ARG	329	21.659	0.380	55.701	1.00	18.85	B	
ATOM	4945	CA	ARG	329	22.605	-0.648	55.284	1.00	18.48	B	
ATOM	4946	CB	ARG	329	22.644	-0.784	53.756	1.00	21.31	B	
ATOM	4947	CG	ARG	329	23.540	-1.929	53.249	1.00	27.66	B	
ATOM	4948	CD	ARG	329	23.818	-1.771	51.748	1.00	32.45	B	
ATOM	4949	NE	ARG	329	24.651	-2.837	51.190	1.00	38.68	B	
ATOM	4950	CZ	ARG	329	25.871	-3.147	51.626	1.00	43.03	B	
ATOM	4951	NH1	ARG	329	26.417	-2.476	52.641	1.00	45.11	B	
ATOM	4952	NH2	ARG	329	26.553	-4.122	51.032	1.00	45.04	B	
ATOM	4953	C	ARG	329	23.937	-0.161	55.840	1.00	14.99	B	
ATOM	4954	O	ARG	329	24.361	0.948	55.568	1.00	16.21	B	
ATOM	4955	N	THR	330	24.595	-0.987	56.632	1.00	12.23	B	
ATOM	4956	CA	THR	330	25.842	-0.559	57.235	1.00	11.36	B	
ATOM	4957	CB	THR	330	25.720	-0.515	58.801	1.00	11.85	B	
ATOM	4958	OG1	THR	330	24.663	0.378	59.185	1.00	12.21	B	
ATOM	4959	CG2	THR	330	27.022	-0.038	59.432	1.00	10.17	B	
ATOM	4960	C	THR	330	27.031	-1.424	56.857	1.00	11.32	B	
ATOM	4961	O	THR	330	26.909	-2.639	56.699	1.00	11.14	B	
ATOM	4962	N	SER	331	28.176	-0.760	56.722	1.00	10.11	B	
ATOM	4963	CA	SER	331	29.432	-1.390	56.396	1.00	9.70	B	
ATOM	4964	CB	SER	331	29.762	-1.121	54.938	1.00	10.15	B	
ATOM	4965	OG	SER	331	29.612	-2.305	54.201	1.00	16.41	B	
ATOM	4966	C	SER	331	30.551	-0.861	57.292	1.00	8.79	B	
ATOM	4967	O	SER	331	30.612	0.314	57.575	1.00	10.25	B	
ATOM	4968	N	ILE	332	31.421	-1.744	57.761	1.00	7.54	B	
ATOM	4969	CA	ILE	332	32.537	-1.309	58.580	1.00	5.00	B	
ATOM	4970	CB	ILE	332	32.484	-1.896	59.997	1.00	3.72	B	
ATOM	4971	CG2	ILE	332	33.791	-1.623	60.719	1.00	1.00	B	
ATOM	4972	CG1	ILE	332	31.296	-1.308	60.755	1.00	1.20	B	
ATOM	4973	CD1	ILE	332	31.044	-1.996	62.080	1.00	1.00	B	
ATOM	4974	C	ILE	332	33.825	-1.761	57.915	1.00	6.57	B	
ATOM	4975	O	ILE	332	33.959	-2.921	57.505	1.00	6.08	B	
ATOM	4976	N	ILE	333	34.754	-0.824	57.779	1.00	6.74	B	
ATOM	4977	CA	ILE	333	36.052	-1.110	57.203	1.00	7.94	B	
ATOM	4978	CB	ILE	333	36.377	-0.134	56.043	1.00	7.86	B	
ATOM	4979	CG2	ILE	333	37.745	-0.446	55.482	1.00	10.20	B	
ATOM	4980	CG1	ILE	333	35.335	-0.292	54.935	1.00	9.26	B	
ATOM	4981	CD1	ILE	333	35.562	0.532	53.743	1.00	9.53	B	
ATOM	4982	C	ILE	333	37.050	-0.961	58.362	1.00	9.22	B	
ATOM	4983	O	ILE	333	37.318	0.139	58.833	1.00	9.93	B	
ATOM	4984	N	ALA	334	37.568	-2.087	58.842	1.00	9.27	B	
ATOM	4985	CA	ALA	334	38.510	-2.064	59.950	1.00	9.36	B	
ATOM	4986	CB	ALA	334	38.318	-3.281	60.815	1.00	8.99	B	
ATOM	4987	C	ALA	334	39.914	-2.033	59.366	1.00	9.97	B	
ATOM	4988	O	ALA	334	40.289	-2.887	58.558	1.00	9.97	B	
ATOM	4989	N	THR	335	40.689	-1.039	59.780	1.00	10.59	B	
ATOM	4990	CA	THR	335	42.041	-0.877	59.267	1.00	11.33	B	
ATOM	4991	CB	THR	335	42.300	0.587	58.833	1.00	11.54	B	
ATOM	4992	OG1	THR	335	42.165	1.471	59.959	1.00	11.31	B	
ATOM	4993	CG2	THR	335	41.316	0.973	57.707	1.00	10.89	B	
ATOM	4994	C	THR	335	43.059	-1.311	60.297	1.00	11.80	B	
ATOM	4995	O	THR	335	42.898	-1.044	61.479	1.00	11.91	B	
ATOM	4996	N	ILE	336	44.108	-1.981	59.825	1.00	10.99	B	
ATOM	4997	CA	ILE	336	45.150	-2.494	60.691	1.00	9.23	B	
ATOM	4998	CB	ILE	336	44.988	-4.002	60.867	1.00	6.21	B	
ATOM	4999	CG2	ILE	336	43.726	-4.275	61.631	1.00	2.30	B	
ATOM	5000	CG1	ILE	336	44.949	-4.688	59.501	1.00	4.99	B	
ATOM	5001	CD1	ILE	336	44.977	-6.187	59.570	1.00	4.80	B	
ATOM	5002	C	ILE	336	46.549	-2.201	60.175	1.00	12.29	B	
ATOM	5003	O	ILE	336	46.722	-1.683	59.054	1.00	12.52	B	
ATOM	5004	N	SER	337	47.536	-2.533	61.011	1.00	15.10	B	
ATOM	5005	CA	SER	337	48.958	-2.344	60.716	1.00	17.38	B	
ATOM	5006	CB	SER	337	49.673	-1.619	61.848	1.00	16.32	B	
ATOM	5007	OG	SER	337	51.071	-1.842	61.757	1.00	15.90	B	

ATOM	5008	C	SER	337	49.690	-3.686	60.569	1.00	18.53	B
ATOM	5009	O	SER	337	49.393	-4.652	61.292	1.00	19.54	B
ATOM	5010	N	PRO	338	50.643	-3.770	59.618	1.00	17.27	B
ATOM	5011	CD	PRO	338	50.949	-2.790	58.555	1.00	15.95	B
ATOM	5012	CA	PRO	338	51.398	-5.005	59.403	1.00	15.90	B
ATOM	5013	CB	PRO	338	51.851	-4.868	57.953	1.00	14.63	B
ATOM	5014	CG	PRO	338	52.158	-3.420	57.858	1.00	15.30	B
ATOM	5015	C	PRO	338	52.574	-5.124	60.360	1.00	15.45	B
ATOM	5016	O	PRO	338	53.206	-6.145	60.420	1.00	15.18	B
ATOM	5017	N	ALA	339	52.844	-4.053	61.103	1.00	16.79	B
ATOM	5018	CA	ALA	339	53.986	-3.999	62.025	1.00	19.03	B
ATOM	5019	CB	ALA	339	54.296	-2.536	62.409	1.00	17.80	B
ATOM	5020	C	ALA	339	53.813	-4.824	63.277	1.00	19.74	B
ATOM	5021	O	ALA	339	52.727	-4.883	63.824	1.00	21.39	B
ATOM	5022	N	SER	340	54.896	-5.452	63.734	1.00	20.20	B
ATOM	5023	CA	SER	340	54.825	-6.278	64.940	1.00	20.54	B
ATOM	5024	CB	SER	340	56.045	-7.193	65.075	1.00	21.46	B
ATOM	5025	OG	SER	340	57.233	-6.430	65.182	1.00	24.93	B
ATOM	5026	C	SER	340	54.727	-5.453	66.208	1.00	19.22	B
ATOM	5027	O	SER	340	54.293	-5.941	67.224	1.00	17.09	B
ATOM	5028	N	LEU	341	55.131	-4.191	66.143	1.00	20.29	B
ATOM	5029	CA	LEU	341	55.048	-3.345	67.328	1.00	21.64	B
ATOM	5030	CB	LEU	341	56.040	-2.184	67.248	1.00	23.99	B
ATOM	5031	CG	LEU	341	55.610	-0.896	66.546	1.00	27.23	B
ATOM	5032	CD1	LEU	341	55.641	0.269	67.554	1.00	26.67	B
ATOM	5033	CD2	LEU	341	56.542	-0.630	65.357	1.00	28.22	B
ATOM	5034	C	LEU	341	53.629	-2.807	67.502	1.00	21.40	B
ATOM	5035	O	LEU	341	53.350	-2.053	68.424	1.00	21.64	B
ATOM	5036	N	ASN	342	52.736	-3.227	66.613	1.00	21.16	B
ATOM	5037	CA	ASN	342	51.335	-2.815	66.664	1.00	21.98	B
ATOM	5038	CB	ASN	342	50.943	-2.165	65.352	1.00	20.54	B
ATOM	5039	CG	ASN	342	51.586	-0.826	65.172	1.00	21.64	B
ATOM	5040	OD1	ASN	342	51.897	-0.423	64.046	1.00	19.82	B
ATOM	5041	ND2	ASN	342	51.785	-0.107	66.285	1.00	20.76	B
ATOM	5042	C	ASN	342	50.415	-4.011	66.892	1.00	22.33	B
ATOM	5043	O	ASN	342	49.201	-3.909	66.761	1.00	22.21	B
ATOM	5044	N	LEU	343	51.023	-5.135	67.254	1.00	23.56	B
ATOM	5045	CA	LEU	343	50.334	-6.406	67.488	1.00	24.35	B
ATOM	5046	CB	LEU	343	51.360	-7.435	67.992	1.00	25.91	B
ATOM	5047	CG	LEU	343	50.986	-8.890	68.316	1.00	28.30	B
ATOM	5048	CD1	LEU	343	50.524	-8.995	69.761	1.00	29.51	B
ATOM	5049	CD2	LEU	343	49.930	-9.392	67.334	1.00	28.29	B
ATOM	5050	C	LEU	343	49.119	-6.347	68.412	1.00	22.80	B
ATOM	5051	O	LEU	343	48.024	-6.756	68.045	1.00	21.40	B
ATOM	5052	N	GLU	344	49.305	-5.831	69.614	1.00	23.08	B
ATOM	5053	CA	GLU	344	48.189	-5.745	70.545	1.00	22.34	B
ATOM	5054	CB	GLU	344	48.628	-5.122	71.861	1.00	24.68	B
ATOM	5055	CG	GLU	344	47.491	-4.875	72.821	1.00	30.10	B
ATOM	5056	CD	GLU	344	47.965	-4.715	74.263	1.00	34.59	B
ATOM	5057	OE1	GLU	344	48.866	-3.886	74.538	1.00	36.85	B
ATOM	5058	OE2	GLU	344	47.422	-5.428	75.134	1.00	36.33	B
ATOM	5059	C	GLU	344	47.002	-4.960	70.002	1.00	19.86	B
ATOM	5060	O	GLU	344	45.894	-5.425	70.097	1.00	20.25	B
ATOM	5061	N	GLU	345	47.241	-3.770	69.452	1.00	17.13	B
ATOM	5062	CA	GLU	345	46.141	-2.974	68.907	1.00	16.35	B
ATOM	5063	CB	GLU	345	46.585	-1.527	68.589	1.00	15.68	B
ATOM	5064	CG	GLU	345	46.803	-0.645	69.824	1.00	13.57	B
ATOM	5065	CD	GLU	345	45.528	-0.391	70.618	1.00	13.00	B
ATOM	5066	OE1	GLU	345	45.623	0.062	71.768	1.00	14.32	B
ATOM	5067	OE2	GLU	345	44.419	-0.628	70.111	1.00	13.44	B
ATOM	5068	C	GLU	345	45.528	-3.626	67.659	1.00	14.78	B
ATOM	5069	O	GLU	345	44.326	-3.544	67.442	1.00	14.79	B
ATOM	5070	N	THR	346	46.350	-4.284	66.846	1.00	14.54	B
ATOM	5071	CA	THR	346	45.863	-4.959	65.641	1.00	14.71	B
ATOM	5072	CB	THR	346	47.046	-5.572	64.839	1.00	15.75	B
ATOM	5073	OG1	THR	346	47.870	-4.523	64.301	1.00	19.38	B
ATOM	5074	CG2	THR	346	46.520	-6.467	63.721	1.00	15.93	B
ATOM	5075	C	THR	346	44.888	-6.075	66.057	1.00	14.75	B
ATOM	5076	O	THR	346	43.863	-6.320	65.403	1.00	12.97	B
ATOM	5077	N	LEU	347	45.210	-6.741	67.165	1.00	15.11	B
ATOM	5078	CA	LEU	347	44.371	-7.819	67.693	1.00	14.94	B
ATOM	5079	CB	LEU	347	45.080	-8.601	68.797	1.00	13.17	B
ATOM	5080	CG	LEU	347	46.253	-9.465	68.342	1.00	12.75	B

ATOM	5081	CD1	LEU	347	46.845	-10.156	69.559	1.00	9.82	B	
ATOM	5082	CD2	LEU	347	45.781	-10.459	67.281	1.00	10.19	B	
ATOM	5083	C	LEU	347	43.074	-7.289	68.277	1.00	14.55	B	
ATOM	5084	O	LEU	347	42.039	-7.935	68.196	1.00	16.59	B	
ATOM	5085	N	SER	348	43.127	-6.107	68.872	1.00	14.94	B	
ATOM	5086	CA	SER	348	41.917	-5.534	69.425	1.00	12.88	B	
ATOM	5087	CB	SER	348	42.236	-4.288	70.204	1.00	11.62	B	
ATOM	5088	OG	SER	348	42.841	-4.656	71.416	1.00	18.29	B	
ATOM	5089	C	SER	348	40.974	-5.180	68.303	1.00	12.87	B	
ATOM	5090	O	SER	348	39.809	-5.505	68.355	1.00	12.88	B	
ATOM	5091	N	THR	349	41.494	-4.518	67.281	1.00	12.34	B	
ATOM	5092	CA	THR	349	40.672	-4.121	66.151	1.00	14.07	B	
ATOM	5093	CB	THR	349	41.515	-3.400	65.081	1.00	14.87	B	
ATOM	5094	OG1	THR	349	41.887	-2.096	65.535	1.00	17.94	B	
ATOM	5095	CG2	THR	349	40.738	-3.238	63.828	1.00	15.48	B	
ATOM	5096	C	THR	349	39.992	-5.321	65.493	1.00	16.16	B	
ATOM	5097	O	THR	349	38.770	-5.325	65.282	1.00	15.82	B	
ATOM	5098	N	LEU	350	40.777	-6.339	65.157	1.00	15.00	B	
ATOM	5099	CA	LEU	350	40.226	-7.518	64.508	1.00	15.08	B	
ATOM	5100	CB	LEU	350	41.352	-8.496	64.206	1.00	14.08	B	
ATOM	5101	CG	LEU	350	41.963	-8.503	62.812	1.00	10.95	B	
ATOM	5102	CD1	LEU	350	42.004	-7.143	62.214	1.00	10.81	B	
ATOM	5103	CD2	LEU	350	43.347	-9.038	62.947	1.00	11.99	B	
ATOM	5104	C	LEU	350	39.162	-8.172	65.367	1.00	16.48	B	
ATOM	5105	O	LEU	350	38.132	-8.595	64.876	1.00	17.28	B	
ATOM	5106	N	GLU	351	39.443	-8.254	66.658	1.00	18.22	B	
ATOM	5107	CA	GLU	351	38.514	-8.842	67.609	1.00	19.87	B	
ATOM	5108	CB	GLU	351	39.144	-8.846	69.003	1.00	21.84	B	
ATOM	5109	CG	GLU	351	38.494	-9.791	69.965	1.00	26.42	B	
ATOM	5110	CD	GLU	351	38.420	-11.196	69.403	1.00	30.21	B	
ATOM	5111	OE1	GLU	351	39.481	-11.771	69.051	1.00	29.53	B	
ATOM	5112	OE2	GLU	351	37.289	-11.724	69.309	1.00	32.89	B	
ATOM	5113	C	GLU	351	37.217	-8.024	67.646	1.00	19.18	B	
ATOM	5114	O	GLU	351	36.126	-8.569	67.714	1.00	19.57	B	
ATOM	5115	N	TYR	352	37.368	-6.703	67.603	1.00	18.87	B	
ATOM	5116	CA	TYR	352	36.258	-5.756	67.646	1.00	17.30	B	
ATOM	5117	CB	TYR	352	36.816	-4.348	67.891	1.00	14.25	B	
ATOM	5118	CG	TYR	352	35.794	-3.239	68.039	1.00	11.72	B	
ATOM	5119	CD1	TYR	352	35.105	-2.729	66.933	1.00	11.26	B	
ATOM	5120	CE1	TYR	352	34.220	-1.649	67.067	1.00	11.17	B	
ATOM	5121	CD2	TYR	352	35.570	-2.654	69.282	1.00	10.15	B	
ATOM	5122	CE2	TYR	352	34.699	-1.584	69.433	1.00	9.37	B	
ATOM	5123	CZ	TYR	352	34.024	-1.078	68.322	1.00	11.62	B	
ATOM	5124	OH	TYR	352	33.175	0.010	68.445	1.00	14.22	B	
ATOM	5125	C	TYR	352	35.442	-5.814	66.362	1.00	18.80	B	
ATOM	5126	O	TYR	352	34.217	-5.852	66.407	1.00	19.93	B	
ATOM	5127	N	ALA	353	36.115	-5.822	65.216	1.00	18.33	B	
ATOM	5128	CA	ALA	353	35.406	-5.891	63.951	1.00	17.31	B	
ATOM	5129	CB	ALA	353	36.359	-5.698	62.821	1.00	16.39	B	
ATOM	5130	C	ALA	353	34.680	-7.221	63.785	1.00	18.36	B	
ATOM	5131	O	ALA	353	33.542	-7.249	63.365	1.00	18.10	B	
ATOM	5132	N	HIS	354	35.354	-8.319	64.119	1.00	19.39	B	
ATOM	5133	CA	HIS	354	34.779	-9.661	63.994	1.00	20.34	B	
ATOM	5134	CB	HIS	354	35.761	-10.712	64.509	1.00	22.75	B	
ATOM	5135	CG	HIS	354	35.302	-12.121	64.294	1.00	25.34	B	
ATOM	5136	CD2	HIS	354	34.797	-13.031	65.156	1.00	25.57	B	
ATOM	5137	ND1	HIS	354	35.311	-12.725	63.053	1.00	25.77	B	
ATOM	5138	CE1	HIS	354	34.831	-13.948	63.164	1.00	26.03	B	
ATOM	5139	NE2	HIS	354	34.511	-14.162	64.427	1.00	26.67	B	
ATOM	5140	C	HIS	354	33.486	-9.811	64.796	1.00	20.23	B	
ATOM	5141	O	HIS	354	32.512	-10.417	64.352	1.00	18.53	B	
ATOM	5142	N	ARG	355	33.505	-9.255	65.995	1.00	20.24	B	
ATOM	5143	CA	ARG	355	32.370	-9.285	66.891	1.00	20.90	B	
ATOM	5144	CB	ARG	355	32.823	-8.721	68.239	1.00	20.70	B	
ATOM	5145	CG	ARG	355	31.789	-8.672	69.339	1.00	21.77	B	
ATOM	5146	CD	ARG	355	32.433	-8.121	70.598	1.00	22.76	B	
ATOM	5147	NE	ARG	355	31.461	-7.943	71.673	1.00	27.66	B	
ATOM	5148	CZ	ARG	355	30.820	-8.942	72.281	1.00	31.26	B	
ATOM	5149	NH1	ARG	355	31.042	-10.206	71.921	1.00	31.17	B	
ATOM	5150	NH2	ARG	355	29.965	-8.679	73.262	1.00	31.12	B	
ATOM	5151	C	ARG	355	31.177	-8.513	66.305	1.00	21.80	B	
ATOM	5152	O	ARG	355	30.040	-8.932	66.453	1.00	23.53	B	
ATOM	5153	N	ALA	356	31.442	-7.394	65.634	1.00	21.31	B	

ATOM	5154	CA	ALA	356	30.375	-6.586	65.049	1.00	20.41	B
ATOM	5155	CB	ALA	356	30.924	-5.282	64.583	1.00	20.58	B
ATOM	5156	C	ALA	356	29.618	-7.256	63.902	1.00	20.99	B
ATOM	5157	O	ALA	356	28.531	-6.796	63.543	1.00	19.69	B
ATOM	5158	N	LYS	357	30.195	-8.328	63.340	1.00	22.58	B
ATOM	5159	CA	LYS	357	29.590	-9.081	62.225	1.00	22.82	B
ATOM	5160	CB	LYS	357	30.347	-10.371	61.911	1.00	23.14	B
ATOM	5161	CG	LYS	357	31.767	-10.194	61.443	1.00	25.46	B
ATOM	5162	CD	LYS	357	31.897	-10.597	59.983	1.00	27.85	B
ATOM	5163	CE	LYS	357	31.660	-12.104	59.763	1.00	27.26	B
ATOM	5164	NZ	LYS	357	32.648	-12.966	60.485	1.00	27.32	B
ATOM	5165	C	LYS	357	28.198	-9.551	62.594	1.00	23.74	B
ATOM	5166	O	LYS	357	27.315	-9.635	61.755	1.00	22.43	B
ATOM	5167	N	ASN	358	28.016	-9.845	63.876	1.00	25.58	B
ATOM	5168	CA	ASN	358	26.730	-10.306	64.388	1.00	28.23	B
ATOM	5169	CB	ASN	358	26.914	-10.928	65.766	1.00	28.39	B
ATOM	5170	CG	ASN	358	27.852	-12.105	65.742	1.00	29.97	B
ATOM	5171	OD1	ASN	358	28.203	-12.649	66.778	1.00	31.69	B
ATOM	5172	ND2	ASN	358	28.267	-12.506	64.551	1.00	29.57	B
ATOM	5173	C	ASN	358	25.606	-9.270	64.476	1.00	30.00	B
ATOM	5174	O	ASN	358	24.487	-9.619	64.845	1.00	30.93	B
ATOM	5175	N	ILE	359	25.892	-8.011	64.152	1.00	31.11	B
ATOM	5176	CA	ILE	359	24.855	-6.986	64.176	1.00	32.09	B
ATOM	5177	CB	ILE	359	25.465	-5.604	64.142	1.00	31.91	B
ATOM	5178	CG2	ILE	359	24.367	-4.569	64.136	1.00	30.39	B
ATOM	5179	CG1	ILE	359	26.375	-5.433	65.361	1.00	32.12	B
ATOM	5180	CD1	ILE	359	27.169	-4.134	65.382	1.00	34.29	B
ATOM	5181	C	ILE	359	23.903	-7.152	62.984	1.00	33.89	B
ATOM	5182	O	ILE	359	24.326	-7.355	61.843	1.00	32.83	B
ATOM	5183	N	LEU	360	22.605	-7.080	63.256	1.00	36.27	B
ATOM	5184	CA	LEU	360	21.597	-7.249	62.211	1.00	39.23	B
ATOM	5185	CB	LEU	360	20.630	-8.381	62.583	1.00	42.29	B
ATOM	5186	CG	LEU	360	19.497	-8.742	61.609	1.00	44.94	B
ATOM	5187	CD1	LEU	360	20.073	-9.122	60.240	1.00	44.70	B
ATOM	5188	CD2	LEU	360	18.676	-9.901	62.188	1.00	45.24	B
ATOM	5189	C	LEU	360	20.800	-5.970	62.028	1.00	39.70	B
ATOM	5190	O	LEU	360	20.286	-5.429	62.994	1.00	39.55	B
ATOM	5191	N	ASN	361	20.710	-5.509	60.777	1.00	40.33	B
ATOM	5192	CA	ASN	361	19.989	-4.286	60.413	1.00	39.80	B
ATOM	5193	CB	ASN	361	20.865	-3.358	59.573	1.00	40.62	B
ATOM	5194	CG	ASN	361	22.050	-2.798	60.350	1.00	41.69	B
ATOM	5195	OD1	ASN	361	22.893	-2.087	59.792	1.00	41.21	B
ATOM	5196	ND2	ASN	361	22.119	-3.109	61.633	1.00	41.78	B
ATOM	5197	C	ASN	361	18.748	-4.575	59.575	1.00	40.40	B
ATOM	5198	O	ASN	361	18.630	-5.637	58.974	1.00	41.33	B
ATOM	5199	N	LYS	362	17.838	-3.604	59.535	1.00	40.64	B
ATOM	5200	CA	LYS	362	16.572	-3.687	58.795	1.00	40.39	B
ATOM	5201	CB	LYS	362	16.811	-3.781	57.283	1.00	38.42	B
ATOM	5202	CG	LYS	362	17.283	-2.481	56.664	1.00	37.04	B
ATOM	5203	CD	LYS	362	17.312	-2.553	55.151	1.00	35.58	B
ATOM	5204	CE	LYS	362	15.915	-2.479	54.570	1.00	35.06	B
ATOM	5205	NZ	LYS	362	15.248	-1.182	54.828	1.00	33.80	B
ATOM	5206	C	LYS	362	15.654	-4.833	59.222	1.00	40.02	B
ATOM	5207	O	LYS	362	15.341	-5.705	58.378	1.00	41.01	B
ATOM	5208	OXT	LYS	362	15.244	-4.848	60.404	1.00	38.46	B
ATOM	5209	MG	MG	2602	43.447	10.556	59.883	1.00	1.46	
ATOM	5238	PB	ADP	2600	44.598	7.110	60.307	1.00	12.39	ADP
ATOM	5239	O1B	ADP	2600	45.185	7.724	61.540	1.00	6.06	ADP
ATOM	5240	O2B	ADP	2600	44.098	5.627	60.595	1.00	9.47	ADP
ATOM	5241	O3B	ADP	2600	43.494	7.932	59.799	1.00	9.32	ADP
ATOM	5242	PA	ADP	2600	45.933	7.683	57.885	1.00	15.76	ADP
ATOM	5243	O1A	ADP	2600	44.910	7.319	56.926	1.00	19.46	ADP
ATOM	5244	O2A	ADP	2600	45.886	9.129	58.130	1.00	18.59	ADP
ATOM	5245	O3A	ADP	2600	45.669	6.908	59.185	1.00	14.04	ADP
ATOM	5246	O5*	ADP	2600	47.412	7.404	57.328	1.00	19.34	ADP
ATOM	5247	C5*	ADP	2600	48.489	6.585	57.824	1.00	22.53	ADP
ATOM	5248	C4*	ADP	2600	49.691	6.801	56.820	1.00	24.49	ADP
ATOM	5249	O4*	ADP	2600	49.780	5.604	56.098	1.00	26.34	ADP
ATOM	5250	C3*	ADP	2600	49.504	7.928	55.757	1.00	24.13	ADP
ATOM	5251	O3*	ADP	2600	50.670	8.755	55.611	1.00	26.52	ADP
ATOM	5252	C2*	ADP	2600	49.154	7.243	54.456	1.00	25.11	ADP
ATOM	5253	O2*	ADP	2600	49.698	7.905	53.303	1.00	27.28	ADP
ATOM	5254	C1*	ADP	2600	49.652	5.829	54.676	1.00	26.94	ADP

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ATOM   5255  N9  ADP  2600      48.736   4.765  54.191  1.00 27.64      ADP
ATOM   5256  C8  ADP  2600      47.767   4.193  54.941  1.00 26.96      ADP
ATOM   5257  N7  ADP  2600      47.150   3.292  54.228  1.00 29.21      ADP
ATOM   5258  C5  ADP  2600      47.690   3.269  53.027  1.00 29.55      ADP
ATOM   5259  C6  ADP  2600      47.466   2.525  51.857  1.00 29.68      ADP
ATOM   5260  N6  ADP  2600      46.495   1.606  51.861  1.00 29.43      ADP
ATOM   5261  N1  ADP  2600      48.250   2.751  50.704  1.00 30.06      ADP
ATOM   5262  C2  ADP  2600      49.252   3.696  50.678  1.00 29.27      ADP
ATOM   5263  N3  ADP  2600      49.466   4.411  51.827  1.00 29.94      ADP
ATOM   5264  C4  ADP  2600      48.711   4.230  52.991  1.00 28.23      ADP
ATOM   5291  C1  4-2A    1      42.197  14.937  49.097  1.00 25.59      4-2A
ATOM   5292  C2  4-2A    1      41.920  14.433  47.714  1.00 25.74      4-2A
ATOM   5293  C3  4-2A    1      41.044  15.120  46.829  1.00 26.03      4-2A
ATOM   5294  C4  4-2A    1      40.929  14.774  45.500  1.00 26.67      4-2A
ATOM   5295  C5  4-2A    1      41.663  13.715  44.991  1.00 25.62      4-2A
ATOM   5296  C6  4-2A    1      42.514  12.931  45.817  1.00 25.53      4-2A
ATOM   5297  C7  4-2A    1      42.617  13.291  47.201  1.00 25.82      4-2A
ATOM   5298  O12 4-2A    1      43.246  11.914  45.291  1.00 25.59      4-2A
ATOM   5299  C14 4-2A    1      40.974  14.917  49.926  1.00 26.54      4-2A
ATOM   5300  C15 4-2A    1      40.461  16.085  50.528  1.00 26.66      4-2A
ATOM   5301  C16 4-2A    1      41.255  17.420  50.551  1.00 26.17      4-2A
ATOM   5302  C17 4-2A    1      42.265  17.452  49.404  1.00 26.31      4-2A
ATOM   5303  N18 4-2A    1      42.979  16.179  49.355  1.00 26.30      4-2A
ATOM   5304  C22 4-2A    1      43.422  18.425  49.565  1.00 25.84      4-2A
ATOM   5305  N23 4-2A    1      44.551  17.713  49.505  1.00 25.90      4-2A
ATOM   5306  C24 4-2A    1      44.289  16.370  49.394  1.00 26.52      4-2A
ATOM   5307  N26 4-2A    1      40.109  13.877  50.027  1.00 26.97      4-2A
ATOM   5308  C27 4-2A    1      38.991  14.325  50.732  1.00 26.51      4-2A
ATOM   5309  C28 4-2A    1      39.211  15.740  51.093  1.00 27.62      4-2A
ATOM   5310  C29 4-2A    1      37.745  13.725  51.140  1.00 26.04      4-2A
ATOM   5311  C30 4-2A    1      36.783  14.431  51.909  1.00 26.80      4-2A
ATOM   5312  C31 4-2A    1      37.035  15.782  52.312  1.00 27.44      4-2A
ATOM   5313  C32 4-2A    1      38.217  16.439  51.892  1.00 27.46      4-2A
ATOM   5314  O37 4-2A    1      43.236  19.647  49.683  1.00 24.48      4-2A
ATOM   5315  O38 4-2A    1      45.096  15.436  49.375  1.00 27.32      4-2A
ATOM   5316  C39 4-2A    1      45.831  18.372  49.744  1.00 25.80      4-2A
END
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TABLE 5

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REMARK   1 kin_16dpb molecule B
REMARK r= 0.2114 free_r= 0.2639
REMARK rmsd bonds= 0.006712  rmsd angles=  1.32262
REMARK B rmsd for bonded mainchain atoms=  1.570  target= 1.5
REMARK B rmsd for bonded sidechain atoms=  2.570  target= 2.0
REMARK B rmsd for angle mainchain atoms=  2.729  target= 2.0
REMARK B rmsd for angle sidechain atoms=  3.936  target= 2.5
REMARK sg= P2(1)2(1)2(1) a= 69.48 b= 79.54 c= 158.98 alpha= 90. beta= 90. gamma= 90.
REMARK reflection file= k2a.cv
REMARK B-correction resolution: 6.0 - 2.5
REMARK FILENAME="kin_16dpb.pdb"
ATOM    788  N   GLU   116      39.151   9.227  52.663  1.00  8.87      B
ATOM    789  CA  GLU   116      39.430  10.450  51.915  1.00  8.17      B
ATOM    790  CB  GLU   116      39.921  11.534  52.868  1.00  8.92      B
ATOM    791  CG  GLU   116      38.920  11.894  53.939  1.00 12.15      B
ATOM    792  CD  GLU   116      39.349  13.091  54.738  1.00 15.35      B
ATOM    793  OE1 GLU   116      40.362  13.717  54.354  1.00 17.99      B
ATOM    794  OE2 GLU   116      38.678  13.410  55.737  1.00 15.94      B
ATOM    795  C   GLU   116      40.426  10.321  50.784  1.00  8.20      B
ATOM    796  O   GLU   116      40.163  10.736  49.657  1.00  4.89      B
ATOM    797  N   GLY   117      41.577   9.744  51.097  1.00  9.09      B
ATOM    798  CA  GLY   117      42.619   9.608  50.104  1.00 10.26      B
ATOM    799  C   GLY   117      43.531  10.819  50.183  1.00 11.18      B
ATOM    800  O   GLY   117      43.289  11.751  50.951  1.00 10.98      B
ATOM    801  N   GLU   118      44.590  10.813  49.389  1.00 13.18      B
ATOM    802  CA  GLU   118      45.531  11.922  49.386  1.00 14.36      B
ATOM    803  CB  GLU   118      46.849  11.498  50.043  1.00 15.18      B
ATOM    804  CG  GLU   118      46.685  10.756  51.363  1.00 21.23      B
ATOM    805  CD  GLU   118      48.014  10.310  51.970  1.00 24.46      B
ATOM    806  OE1 GLU   118      48.894   9.845  51.215  1.00 27.49      B
ATOM    807  OE2 GLU   118      48.177  10.413  53.205  1.00 26.10      B
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ATOM	808	C	GLU	118	45.770	12.281	47.933	1.00	13.80	B
ATOM	809	O	GLU	118	45.126	11.734	47.041	1.00	14.44	B
ATOM	810	N	ARG	119	46.689	13.201	47.685	1.00	13.24	B
ATOM	811	CA	ARG	119	46.984	13.568	46.315	1.00	14.66	B
ATOM	812	CB	ARG	119	47.120	15.088	46.167	1.00	12.36	B
ATOM	813	CG	ARG	119	45.879	15.905	46.518	1.00	11.10	B
ATOM	814	CD	ARG	119	44.628	15.371	45.842	1.00	12.06	B
ATOM	815	NE	ARG	119	44.829	15.087	44.422	1.00	13.81	B
ATOM	816	CZ	ARG	119	44.750	15.992	43.451	1.00	14.81	B
ATOM	817	NH1	ARG	119	44.464	17.257	43.742	1.00	13.37	B
ATOM	818	NH2	ARG	119	44.964	15.632	42.189	1.00	11.75	B
ATOM	819	C	ARG	119	48.288	12.911	45.889	1.00	16.73	B
ATOM	820	O	ARG	119	49.253	12.857	46.662	1.00	17.59	B
ATOM	879	N	TRP	127	42.371	15.847	40.233	1.00	18.06	B
ATOM	880	CA	TRP	127	41.717	15.171	41.335	1.00	16.78	B
ATOM	881	CB	TRP	127	40.912	16.167	42.178	1.00	14.46	B
ATOM	882	CG	TRP	127	39.646	16.618	41.539	1.00	10.93	B
ATOM	883	CD2	TRP	127	38.365	15.996	41.664	1.00	8.71	B
ATOM	884	CE2	TRP	127	37.452	16.770	40.915	1.00	9.40	B
ATOM	885	CE3	TRP	127	37.901	14.857	42.334	1.00	7.23	B
ATOM	886	CD1	TRP	127	39.474	17.709	40.738	1.00	10.58	B
ATOM	887	NE1	TRP	127	38.153	17.810	40.361	1.00	8.88	B
ATOM	888	CZ2	TRP	127	36.095	16.446	40.820	1.00	9.55	B
ATOM	889	CZ3	TRP	127	36.545	14.526	42.242	1.00	9.73	B
ATOM	890	CH2	TRP	127	35.659	15.324	41.488	1.00	11.69	B
ATOM	891	C	TRP	127	40.828	14.002	40.941	1.00	17.94	B
ATOM	892	O	TRP	127	40.817	12.978	41.621	1.00	18.94	B
ATOM	911	N	ASP	130	43.130	10.872	40.183	1.00	18.67	B
ATOM	912	CA	ASP	130	44.174	10.489	41.121	1.00	17.72	B
ATOM	913	CB	ASP	130	44.298	11.534	42.229	1.00	15.27	B
ATOM	914	CG	ASP	130	45.675	11.545	42.859	1.00	16.56	B
ATOM	915	OD1	ASP	130	46.157	10.473	43.285	1.00	15.04	B
ATOM	916	OD2	ASP	130	46.277	12.634	42.930	1.00	16.73	B
ATOM	917	C	ASP	130	43.921	9.115	41.733	1.00	16.61	B
ATOM	918	O	ASP	130	42.931	8.905	42.430	1.00	19.40	B
ATOM	926	N	LEU	132	45.069	7.791	44.240	1.00	15.09	B
ATOM	927	CA	LEU	132	45.118	7.772	45.703	1.00	13.40	B
ATOM	928	CB	LEU	132	46.379	8.487	46.227	1.00	10.29	B
ATOM	929	CG	LEU	132	47.765	7.870	45.930	1.00	14.23	B
ATOM	930	CD1	LEU	132	48.877	8.709	46.609	1.00	8.52	B
ATOM	931	CD2	LEU	132	47.829	6.414	46.429	1.00	11.00	B
ATOM	932	C	LEU	132	43.858	8.395	46.310	1.00	12.82	B
ATOM	933	O	LEU	132	43.719	8.473	47.534	1.00	11.90	B
ATOM	934	N	ALA	133	42.936	8.833	45.457	1.00	12.47	B
ATOM	935	CA	ALA	133	41.681	9.414	45.936	1.00	12.78	B
ATOM	936	CB	ALA	133	40.826	9.884	44.755	1.00	11.66	B
ATOM	937	C	ALA	133	40.928	8.356	46.742	1.00	13.76	B
ATOM	938	O	ALA	133	40.991	7.163	46.431	1.00	13.92	B
ATOM	939	N	GLY	134	40.217	8.798	47.776	1.00	14.68	B
ATOM	940	CA	GLY	134	39.483	7.870	48.619	1.00	13.15	B
ATOM	941	C	GLY	134	38.016	7.752	48.262	1.00	14.05	B
ATOM	942	O	GLY	134	37.574	8.262	47.228	1.00	12.84	B
ATOM	951	N	ILE	136	35.223	9.141	49.530	1.00	10.60	B
ATOM	952	CA	ILE	136	34.466	10.377	49.379	1.00	10.62	B
ATOM	953	CB	ILE	136	34.843	11.386	50.482	1.00	10.47	B
ATOM	954	CG2	ILE	136	34.175	12.721	50.231	1.00	8.18	B
ATOM	955	CG1	ILE	136	34.382	10.847	51.839	1.00	10.73	B
ATOM	956	CD1	ILE	136	34.760	11.746	53.047	1.00	13.23	B
ATOM	957	C	ILE	136	34.553	11.030	47.995	1.00	11.05	B
ATOM	958	O	ILE	136	33.531	11.296	47.373	1.00	10.67	B
ATOM	959	N	PRO	137	35.765	11.303	47.492	1.00	11.64	B
ATOM	960	CD	PRO	137	37.100	11.313	48.114	1.00	11.30	B
ATOM	961	CA	PRO	137	35.793	11.924	46.162	1.00	11.06	B
ATOM	962	CB	PRO	137	37.237	12.410	46.031	1.00	10.03	B
ATOM	963	CG	PRO	137	38.002	11.469	46.911	1.00	11.65	B
ATOM	964	C	PRO	137	35.369	10.997	45.019	1.00	11.97	B
ATOM	965	O	PRO	137	34.867	11.455	43.989	1.00	11.71	B
ATOM	1145	N	LEU	160	29.446	18.027	56.397	1.00	13.49	B
ATOM	1146	CA	LEU	160	30.595	17.478	57.077	1.00	13.18	B
ATOM	1147	CB	LEU	160	31.883	18.025	56.470	1.00	14.21	B
ATOM	1148	CG	LEU	160	33.175	17.477	57.068	1.00	13.62	B
ATOM	1149	CD1	LEU	160	33.056	15.961	57.243	1.00	13.33	B
ATOM	1150	CD2	LEU	160	34.343	17.846	56.166	1.00	13.39	B

ATOM	1151	C	LEU	160	30.492	17.857	58.543	1.00	13.90	B
ATOM	1152	O	LEU	160	30.883	18.956	58.947	1.00	11.88	B
ATOM	1564	N	TYR	211	35.581	19.271	44.173	1.00	18.55	B
ATOM	1565	CA	TYR	211	36.924	19.418	44.731	1.00	18.51	B
ATOM	1566	CB	TYR	211	37.994	19.405	43.637	1.00	15.05	B
ATOM	1567	CG	TYR	211	39.385	19.255	44.201	1.00	14.52	B
ATOM	1568	CD1	TYR	211	39.721	18.153	44.981	1.00	15.06	B
ATOM	1569	CE1	TYR	211	40.989	18.023	45.540	1.00	14.43	B
ATOM	1570	CD2	TYR	211	40.359	20.232	43.988	1.00	13.72	B
ATOM	1571	CE2	TYR	211	41.629	20.112	44.541	1.00	12.86	B
ATOM	1572	CZ	TYR	211	41.937	19.003	45.316	1.00	13.41	B
ATOM	1573	OH	TYR	211	43.192	18.863	45.864	1.00	13.57	B
ATOM	1574	C	TYR	211	37.044	20.683	45.575	1.00	19.47	B
ATOM	1575	O	TYR	211	37.567	20.640	46.688	1.00	21.09	B
ATOM	1593	N	LEU	214	35.512	20.128	48.935	1.00	13.24	B
ATOM	1594	CA	LEU	214	36.304	19.274	49.805	1.00	13.61	B
ATOM	1595	CB	LEU	214	36.778	18.022	49.055	1.00	11.20	B
ATOM	1596	CG	LEU	214	35.695	17.141	48.423	1.00	12.16	B
ATOM	1597	CD1	LEU	214	36.340	15.933	47.756	1.00	10.83	B
ATOM	1598	CD2	LEU	214	34.703	16.686	49.485	1.00	11.84	B
ATOM	1599	C	LEU	214	37.503	20.063	50.332	1.00	14.64	B
ATOM	1600	O	LEU	214	37.903	19.885	51.476	1.00	16.56	B
ATOM	1601	N	GLU	215	38.065	20.946	49.506	1.00	16.42	B
ATOM	1602	CA	GLU	215	39.216	21.748	49.930	1.00	18.40	B
ATOM	1603	CB	GLU	215	39.764	22.595	48.781	1.00	18.89	B
ATOM	1604	CG	GLU	215	40.428	21.819	47.673	1.00	21.62	B
ATOM	1605	CD	GLU	215	40.989	22.739	46.598	1.00	25.34	B
ATOM	1606	OE1	GLU	215	42.227	22.957	46.572	1.00	24.25	B
ATOM	1607	OE2	GLU	215	40.182	23.256	45.788	1.00	24.35	B
ATOM	1608	C	GLU	215	38.856	22.676	51.077	1.00	17.37	B
ATOM	1609	O	GLU	215	39.600	22.779	52.053	1.00	17.62	B
ATOM	1619	N	GLY	217	36.574	22.385	53.343	1.00	17.13	B
ATOM	1620	CA	GLY	217	36.448	21.651	54.586	1.00	16.36	B
ATOM	1621	C	GLY	217	37.821	21.367	55.173	1.00	16.18	B
ATOM	1622	O	GLY	217	38.044	21.542	56.378	1.00	15.76	B
ATOM	1623	N	ALA	218	38.746	20.934	54.322	1.00	15.35	B
ATOM	1624	CA	ALA	218	40.105	20.629	54.763	1.00	15.51	B
ATOM	1625	CB	ALA	218	40.923	20.071	53.596	1.00	14.52	B
ATOM	1626	C	ALA	218	40.806	21.849	55.356	1.00	14.85	B
ATOM	1627	O	ALA	218	41.470	21.745	56.386	1.00	15.80	B
ATOM	1642	N	ARG	221	39.496	22.571	58.714	1.00	13.46	B
ATOM	1643	CA	ARG	221	39.917	21.498	59.606	1.00	14.10	B
ATOM	1644	CB	ARG	221	39.866	20.171	58.853	1.00	13.82	B
ATOM	1645	CG	ARG	221	39.982	18.949	59.723	1.00	18.08	B
ATOM	1646	CD	ARG	221	39.939	17.690	58.874	1.00	19.00	B
ATOM	1647	NE	ARG	221	38.585	17.167	58.725	1.00	18.62	B
ATOM	1648	CZ	ARG	221	38.226	16.296	57.788	1.00	20.44	B
ATOM	1649	NH1	ARG	221	39.122	15.860	56.905	1.00	20.22	B
ATOM	1650	NH2	ARG	221	36.980	15.839	57.751	1.00	16.95	B
ATOM	1651	C	ARG	221	41.331	21.780	60.137	1.00	14.31	B
ATOM	1652	O	ARG	221	41.669	21.408	61.271	1.00	14.60	B
ATOM	1777	N	PHE	239	30.844	12.531	56.963	1.00	10.36	B
ATOM	1778	CA	PHE	239	30.590	13.199	55.695	1.00	10.45	B
ATOM	1779	CB	PHE	239	31.785	13.041	54.753	1.00	10.20	B
ATOM	1780	CG	PHE	239	31.691	13.879	53.513	1.00	7.76	B
ATOM	1781	CD1	PHE	239	30.822	13.533	52.479	1.00	7.06	B
ATOM	1782	CD2	PHE	239	32.466	15.026	53.386	1.00	6.02	B
ATOM	1783	CE1	PHE	239	30.729	14.329	51.327	1.00	7.31	B
ATOM	1784	CE2	PHE	239	32.384	15.829	52.242	1.00	6.13	B
ATOM	1785	CZ	PHE	239	31.516	15.483	51.210	1.00	5.13	B
ATOM	1786	C	PHE	239	29.350	12.555	55.085	1.00	12.53	B
ATOM	1787	O	PHE	239	29.360	11.369	54.734	1.00	12.06	B
ATOM	2624	MG	MG	2602	43.714	10.353	59.884	1.00	13.44	
ATOM	2625	PB	ADP	2600	44.677	7.176	60.125	1.00	9.41	ADP
ATOM	2626	O1B	ADP	2600	45.207	7.814	61.350	1.00	10.96	ADP
ATOM	2627	O2B	ADP	2600	44.169	5.685	60.429	1.00	12.45	ADP
ATOM	2628	O3B	ADP	2600	43.584	7.969	59.545	1.00	8.39	ADP
ATOM	2629	PA	ADP	2600	46.112	7.788	57.787	1.00	12.25	ADP
ATOM	2630	O1A	ADP	2600	45.124	7.466	56.774	1.00	14.66	ADP
ATOM	2631	O2A	ADP	2600	46.054	9.225	58.059	1.00	14.40	ADP
ATOM	2632	O3A	ADP	2600	45.825	7.002	59.093	1.00	9.50	ADP
ATOM	2633	O5*	ADP	2600	47.568	7.490	57.279	1.00	16.91	ADP
ATOM	2634	C5*	ADP	2600	48.603	6.677	57.812	1.00	18.22	ADP

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ATOM   2635  C4* ADP  2600      49.807   6.826  56.807  1.00 21.00      ADP
ATOM   2636  O4* ADP  2600      49.837   5.609  56.073  1.00 23.65      ADP
ATOM   2637  C3* ADP  2600      49.662   7.936  55.733  1.00 20.88      ADP
ATOM   2638  O3* ADP  2600      50.883   8.668  55.538  1.00 23.91      ADP
ATOM   2639  C2* ADP  2600      49.227   7.250  54.452  1.00 21.72      ADP
ATOM   2640  O2* ADP  2600      49.726   7.910  53.286  1.00 24.74      ADP
ATOM   2641  C1* ADP  2600      49.720   5.835  54.648  1.00 22.48      ADP
ATOM   2642  N9   ADP  2600      48.789   4.775  54.145  1.00 22.01      ADP
ATOM   2643  C8   ADP  2600      47.775   4.231  54.861  1.00 22.26      ADP
ATOM   2644  N7   ADP  2600      47.163   3.322  54.140  1.00 24.15      ADP
ATOM   2645  C5   ADP  2600      47.742   3.257  52.980  1.00 24.22      ADP
ATOM   2646  C6   ADP  2600      47.552   2.498  51.838  1.00 25.28      ADP
ATOM   2647  N6   ADP  2600      46.577   1.596  51.801  1.00 26.60      ADP
ATOM   2648  N1   ADP  2600      48.372   2.684  50.738  1.00 28.22      ADP
ATOM   2649  C2   ADP  2600      49.388   3.599  50.736  1.00 27.91      ADP
ATOM   2650  N3   ADP  2600      49.583   4.338  51.852  1.00 25.85      ADP
ATOM   2651  C4   ADP  2600      48.803   4.199  52.972  1.00 23.75      ADP
ATOM   2879  C1   5-2b    1      40.179  14.530  46.990  1.00 27.45      5-2b
ATOM   2880  C2   5-2b    1      41.169  13.921  47.825  1.00 31.74      5-2b
ATOM   2881  C3   5-2b    1      42.197  13.109  47.246  1.00 26.68      5-2b
ATOM   2882  C4   5-2b    1      42.197  12.949  45.832  1.00 25.21      5-2b
ATOM   2883  C5   5-2b    1      41.213  13.549  44.997  1.00 25.57      5-2b
ATOM   2884  C6   5-2b    1      40.174  14.358  45.564  1.00 26.52      5-2b
ATOM   2885  C7   5-2b    1      41.159  14.149  49.287  1.00 39.17      5-2b
ATOM   2886  N8   5-2b    1      40.043  13.644  50.068  1.00 32.24      5-2b
ATOM   2887  C9   5-2b    1      39.077  14.446  50.550  1.00 31.10      5-2b
ATOM   2888  N10  5-2b    1      39.335  15.753  50.627  1.00 35.90      5-2b
ATOM   2889  C11  5-2b    1      40.586  16.353  50.204  1.00 43.34      5-2b
ATOM   2890  C12  5-2b    1      41.575  15.550  49.725  1.00 51.84      5-2b
ATOM   2891  O13  5-2b    1      43.103  12.325  45.318  1.00 22.27      5-2b
ATOM   2892  C14  5-2b    1      43.049  15.950  49.559  1.00 69.59      5-2b
ATOM   2893  O15  5-2b    1      43.510  17.255  49.536  1.00102.78      5-2b
ATOM   2894  C16  5-2b    1      44.900  17.802  49.405  1.00 94.24      5-2b
ATOM   2895  C17  5-2b    1      44.910  19.338  49.209  1.00 96.86      5-2b
ATOM   2896  C18  5-2b    1      40.562  17.864  50.356  1.00 41.39      5-2b
ATOM   2897  O19  5-2b    1      43.806  15.026  49.427  1.00 72.75      5-2b
ATOM   2898  S20  5-2b    1      37.588  13.867  51.069  1.00 18.63      5-2b
END
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WHAT IS CLAIMED IS:

1. A crystallized complex of KSP and a ligand thereof, wherein the relative structural coordinates of the amino acid residues of KSP are as set forth in Table 1 ± the root mean square deviation from the conserved backbone atoms of not more than about 2 Å.

2. The crystallized complex of Claim 1, wherein the relative structural coordinates of the amino acid residues are as set forth in Table 1 ± the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 0.5 Å.

3. The crystallized complex of Claim 1, wherein said ligand binds said KSP at a ligand binding site comprising the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F).

4. A crystallized complex of KSP and a ligand thereof, wherein the relative structural coordinates of the amino acid residues of KSP are as set forth in Table 2 ± the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2 Å.

5. The crystallized complex of Claim 4, wherein the relative structural coordinates of the amino acid residues are as set forth in Table 2 ± the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 0.5 Å.

6. The crystallized complex of Claim 4, wherein said ligand binds said KSP at a ligand binding site comprising the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F).

7. A crystallized complex of KSP and a ligand thereof, wherein the relative structural coordinates of the amino acid residues of KSP are as set forth in Table 3 ± the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2 Å.

8. The crystallized complex of Claim 7, wherein the relative structural coordinates of the amino acid residues are as set forth in Table 3 ± the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 0.5 Å.

9. The crystallized complex of Claim 7, wherein said ligand binds said KSP at a ligand binding site comprising the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F).

10. A crystallized complex of KSP and a ligand thereof, wherein the relative structural coordinates of the amino acid residues of KSP are as set forth in Table 4 ± the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2 Å.

11. The crystallized complex of Claim 10, wherein the relative structural coordinates of the amino acid residues are as set forth in Table 4 ± the root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 0.5 Å.

12. The crystallized complex of Claim 10, wherein said ligand binds said KSP at a ligand binding site comprising the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F).

13. A ligand binding site of a KSP protein comprising the relative structural coordinates set forth in Table 5 ± the root mean square

deviation from the backbone atoms of said amino acids is not more than about 2 Å.

14. The ligand binding site of a KSP protein according to Claim 13 comprising the relative structural coordinates set forth in Table 5 ± the root mean square deviation from the backbone atoms of said amino acids is not more than about 0.5 Å.

15. The ligand binding site of a KSP protein according to Claim 13 comprising the relative structural coordinates of the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F) as set forth in a table selected from a group consisting of Tables 1, 2, 3 and 4, ± the root mean square deviation from the backbone atoms of said amino acids is not more than about 2 Å.

16. An agent which binds to the ligand binding site of Claim 13, wherein said agent is an inhibitor of KSP function, or a pharmaceutically acceptable salt thereof.

17. A composition comprising : (a) an agent according to Claim 16; and (b) a pharmaceutically acceptable carrier.

18. An agent, or a pharmaceutically acceptable salt thereof, which binds to five or more of the KSP amino acid residues selected from the group consisting of 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F), wherein said agent is an inhibitor of KSP function.

19. A method for identifying an agent that interacts with a ligand binding site of human KSP, comprising the steps of:

(a) determining a ligand binding site of KSP from a three-dimensional model of the KSP binding site as set forth in

Table 5, ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å; and

(b) performing computer fitting analysis to identify an agent which interacts with said ligand binding site.

20. A method for identifying an agent that interacts with a ligand binding site of human KSP, comprising the steps of:

(a) determining a ligand binding site of KSP from a three-dimensional model of KSP using the relative structural coordinates of the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F) as set forth in a Table selected from the group of Tables 1, 2, 3 and 4, ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å; and

(b) performing computer fitting analysis to identify an agent which interacts with said ligand binding site.

21. A method for identifying a potential inhibitor of KSP function, comprising the steps of:

(a) obtaining a three-dimensional model of a KSP binding site wherein said model contains the relative structural coordinates of the ligand binding site of KSP from a three-dimensional model of the ligand binding site as set forth in Table 5, ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å;

(b) employing said three-dimensional model to design or select a potential inhibitor; and

(c) synthesizing or obtaining said potential inhibitor.

22. The method according to Claim 21 wherein the potential inhibitor is designed *de novo*.

23. The method of Claim 21, further comprising the steps of:

(d) contacting said potential inhibitor with KSP in the presence of a KSP binding molecule, and

(e) determining the effect the potential inhibitor has on binding between KSP and the KSP binding molecule.

24. A method for identifying a potential inhibitor of KSP function, comprising the steps of:

(a) generating a three-dimensional model of KSP using the relative structural coordinates as set forth in a table selected from Tables 1, 2, 3 and 4, ± a root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å;

(b) employing said three-dimensional model to design or select a potential inhibitor; and

(c) synthesizing or obtaining said potential inhibitor.

25. The method according to Claim 24 wherein the potential inhibitor is designed *de novo*.

26. The method of Claim 24, further comprising the steps of:

(d) contacting said potential inhibitor with KSP in the presence of a KSP binding molecule, and

(e) determining the effect the potential inhibitor has on binding between KSP and the KSP binding molecule.

27. The method of Claim 21, further comprising contacting the potential inhibitor with KSP in the presence of a KSP binding molecule, and determining the effect the potential inhibitor has on binding between KSP and the KSP binding molecule.

28. The method of Claim 21, further comprising contacting the potential inhibitor with KSP in the presence of one or two

KSP substrates selected from ATP and microtubules, and determining the effect the potential inhibitor has on KSP ATPase activity.

29. A potential inhibitor identified by the method of Claim 21, or a pharmaceutically acceptable salt thereof.

30. A method of identifying an inhibitor compound capable of binding to kinesin spindle protein (KSP), said method comprising:

(a) introducing protein coordinates selected from the protein coordinates provided in a table selected from Tables 1, 2, 3 and 4, ± a root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å, into a suitable computer program so as to define a (+)-monastrol ligand binding site conformation, wherein said program displays the three- dimensional structure of the (+)-monastrol ligand binding site;

(b) creating a three dimensional representation of the (+)-monastrol ligand binding site in said computer program;

(c) displaying and superimposing a three dimensional representation of a test compound on the three dimensional representation of the (+)-monastrol ligand binding site;

(d) assessing whether said test compound fits spatially into the (+)-monastrol ligand binding site;

(e) preparing said test compound that fits spatially into the (+)-monastrol ligand binding site;

(f) using said test compound in a biological assay for KSP function; and

(g) determining whether said test compound inhibits KSP function in said assay.

31. A process for identifying a potential anti-mitotic agent which upon binding to a human KSP inhibits cell proliferation, the process comprising the steps of:

(a) obtaining an X-ray diffraction pattern of a human kinesin spindle protein (KSP) crystal, wherein said KSP has been crystallized in the presence of a mixture of at least two potential ligands;

(d) determining whether a ligand/KSP complex is formed by comparing the electron density map calculated from the X-ray diffraction pattern of said KSP crystal to the electron density map calculated from an X-ray diffraction pattern set forth in a table selected from Table 1, 2, 3 and 4; and

(c) determining whether said ligand from said ligand/KSP complex binds to the ligand binding site of said KSP according to Claim 15, such that upon binding to KSP said ligand inhibits cell proliferation.

32. An anti-mitotic agent identified by the process according to Claim 31, or a pharmaceutically acceptable salt thereof.

33. A composition comprising: (a) an anti-mitotic agent identified according to Claim 32; and (b) a pharmaceutically acceptable carrier.

34. A method of identifying a compound that modulates the binding of a ligand to a ligand binding site of a human KSP, said method comprising: modeling test compounds that fit spatially into a KSP ligand binding site using an atomic structural model of a KSP binding site having the relative structural coordinates as set forth in a table selected from the group consisting of Tables 1, 2, 3 and 4 for the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F), ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å; screening the test compounds in an assay characterized by binding of a ligand to the ligand binding site; and identifying a test compound that modulates binding of said ligand to the KSP at its binding site.

35. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecular complex of a compound bound to the ligand binding site of human KSP, said three-dimensional representation comprising the structural coordinates of the KSP as set forth in a table selected from Tables 1-4 or a homologue of said molecular complex, wherein said homologue comprises a binding site that has a root mean square deviation from the backbone atoms of said KSP of not more than about 2.0 Å.

36. A method for identifying an anti-mitotic agent which upon binding to a target human KSP inhibits cell proliferation, the method comprising the steps of:

(a) obtaining a crystal of KSP, where said KSP has been crystallized while exposed to a mixture of at least two potential ligands;

(b) determining whether a ligand/KSP complex is formed in said crystal; and

(c) identifying a potential anti-mitotic agent as one that binds to said KSP at a ligand binding site having the relative structural coordinates as set forth in Table 5 ± the root mean square deviation of not more than about 2.0 Å.

37. An anti-mitotic agent identified by the method according to Claim 36, or a pharmaceutically acceptable salt thereof.

38. A composition comprising: (a) an anti-mitotic agent according to Claim 37; and (b) a pharmaceutically acceptable carrier.

39. A method for determining the three-dimensional structure of a complex of KSP with a ligand thereof, which comprises obtaining X-ray diffraction data for crystals of the complex comprising the

ligand bound to KSP at a ligand binding site; and utilizing said data to define the three-dimensional structure of the complex.

40. A method for evaluating the ability of a chemical entity to associate with a ligand binding site of human KSP or with at least a portion of the site or a complex comprising the KSP binding site; said method comprising the steps of:

(a) employing computational or experimental means to perform a fitting operation between the chemical entity and said ligand binding site of KSP having the relative structural coordinates as set forth in Table 5 ± the root mean square deviation of not more than about 2.0 Å, thereby obtaining data related to said association; and

(b) analyzing the data obtained in step (a) to determine the characteristics of the association between the chemical entity and said KSP or complex.

41. A chemical entity identified by the method of Claim 37, wherein the chemical entity is capable of interfering with the *in vivo* or *in vitro* motor activity of KSP, or a pharmaceutically acceptable salt thereof.

42. A composition comprising: (a) a chemical entity identified according to Claim 38; and (b) a pharmaceutically acceptable carrier.

43. A method for identifying a potential inhibitor of human kinesin spindle protein (KSP), the method comprising the steps of:

(a) providing a three-dimensional structure of a ligand-bound KSP as defined by atomic coordinates set forth in a table selected from a group consisting of Tables 1, 2, 3 and 4 ± the root mean square deviation of not more than about 2.0 Å;

(b) comparing the three-dimensional coordinates of the ligand when it is bound to KSP as set forth in Table 1, 2, 3 or 4 ± the root mean square deviation of not more than about 2.0 Å to the three-dimensional coordinates of a compound in a database of compound structures; and

(c) selecting from said database at least one compound that is structurally similar to said ligand when it is bound to said KSP, wherein the selected compound is a potential inhibitor of said KSP.

44. The method of Claim 43, wherein the structural similarity is determined based on the root mean square deviation in the backbone atoms of the kinesin peptide and the kinesin inhibitor.

45. A method for identifying a potential inhibitor of a human kinesin spindle protein (KSP), the method comprising the steps of:

(a) providing a three-dimensional structure of said KSP as defined by atomic coordinates set forth in a table selected from Tables 1-4 ± the root mean square deviation of not more than about 2.0 Å;

(b) employing the three-dimensional structures to design or select a potential inhibitor;

(c) synthesizing the potential inhibitor; and

(d) contacting the potential inhibitor with KSP to determine the ability of the potential inhibitor to arrest mitosis or inhibit cell proliferation.

46. A potential inhibitor identified by the method of Claim 45 or a pharmaceutically acceptable salt thereof.

47. A composition comprising : (a) the potential inhibitor identified according to Claim 46; and (b) a pharmaceutically acceptable carrier.

48. A method of identifying an inhibitor of KSP wherein the inhibitor binds to the ligand binding site according to Claim 13 which comprises determining the shift in the fluorescence of an amino acid residue at position 127 of KSP, wherein said amino acid residue is tryptophan.

49. The method according to Claim 48 which comprises the steps of:

(a) contacting KSP with the test compound and a nucleotide and measuring the fluorescence of the mixture at the peak emission wavelength for W127 in KSP;

(b) contacting KSP with a nucleotide and measuring the fluorescence of the mixture at the peak emission wavelength for W127 in KSP; and

(c) comparing the fluorescence of the mixture of KSP, the test compound and the nucleotide with the fluorescence of the mixture of KSP with the nucleotide alone.

50. An anti-mitotic agent characterized as:

(a) specifically binding to the target KSP or an analogue thereof at a ligand binding site comprising the relative structural coordinates of the KSP amino acid residues 115 (M), 116(E), 117(G), 118(E), 119(R), 127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P), 160(L) 211(Y), 214(L), 215(E), 217(G), 218(A), 221(R) and 239(F) according to Tables 1, 2, 3 or 4 ± a root mean square deviation from the conserved backbone atoms of said amino acids of not more than about 2.0Å; and

(b) which, upon binding to said KSP or an analogue thereof specifically inhibits said KSP or analogs biological activities.

51. A method of causing the alteration of the structural conformation of a KSP protein which comprises exposing the protein to a ligand that binds to the KSP ligand binding site as set forth in Table 5 ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å.

52. The method according to Claim 51 wherein the KSP protein is additionally bound to a nucleotide.

53. A method of treating or preventing hyper-proliferative diseases which comprises administering to a mammal a therapeutically effective amount of a compound that binds to the KSP ligand binding site as set forth in Table 5 ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2.0 Å.

54. The method according to Claim 53 which is a method of treating or preventing cancer.

55. The method according to Claim 54 which is a method of treating cancer.

56. An isolated and substantially pure polypeptide or a fragment thereof comprising the amino acid sequence as set forth in SEQ ID NO:1.

57. The isolated polypeptide of Claim 56, wherein the polypeptide adopts the conformation of the ligand binding pocket as set forth in Table 5, ± the root mean square deviation of not more than about 2.0 Å.

58. A variant of the isolated polypeptide according to Claim 57 having at least about 80% amino acid sequence identity with the polypeptide of Claim 57, wherein the percentage identity is determined with the algorithm Gap, BASEFIT or FASTA in the Wisconsin Genetics Software Package release 7.0, using default Gap weights.

59. An active structural motif designated herein as pharmacophore model, which refers to the three-dimensional orientation of a set of features describing the physical, chemical and/or electronic environment of the active site of the human KSP, said features comprising either a hydrophobic region feature, a hydrogen bond acceptor feature and a hydrogen bond donor feature (pharmacophore model in FIG. 14A) or two hydrophobic region features and a hydrogen bond acceptor feature (pharmacophore model in FIG. 14B).

60. A method for screening and identifying potential KSP inhibitor compounds by evaluating the fit of the screened compounds to the pharmacophore models of claim 59.

61. The method of claim 60 wherein evaluating the fit is carried out via the use of a computer and a computer-readable medium.

62. A compound, comprising two hydrophobic region features and a hydrogen bond acceptor feature, wherein said features are oriented as illustrated in Figure 14B and wherein said compound inhibits the mitotic kinesin KSP;
or a pharmaceutically acceptable salt thereof.

63. A compound, comprising two hydrophobic region features and a hydrogen bond acceptor feature, wherein said features are oriented as illustrated in Figure 14B and wherein said compound fits within a ligand binding site of a kinesin spindle protein (KSP) protein, said ligand binding site comprising the relative structural coordinates set forth in Table 5 ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2 Å;
or a pharmaceutically acceptable salt thereof.

64. The compound according to Claim 63 wherein the two hydrophobic region features are independently selected from an aryl, heteroaryl and C_3-C_7-cycloalkyl, optionally substituted.

65. The compound according to Claim 63 wherein the two hydrophobic region features are independently selected from an optionally substituted phenyl.

66. The compound according to Claim 63 wherein the compound has a binding affinity for KSP of about 0.1nM to about 100nM.

67. A compound, comprising one hydrophobic region feature, a hydrogen bond donor feature and a hydrogen bond acceptor feature, wherein said

features are oriented as illustrated in Figure 14A and wherein said compound inhibits the mitotic kinesin KSP;

or a pharmaceutically acceptable salt thereof.

68. A compound, comprising one hydrophobic region feature, a hydrogen bond donor feature and a hydrogen bond acceptor feature, wherein said features are oriented as illustrated in Figure 14A and wherein said compound fits within a ligand binding site of a kinesin spindle protein (KSP) protein, said ligand binding site comprising the relative structural coordinates set forth in Table 5 ± the root mean square deviation from the backbone atoms of said amino acids of not more than about 2 Å;

or a pharmaceutically acceptable salt thereof.

69. The compound according to Claim 68 wherein the hydrophobic region feature is selected from an aryl, heteroaryl and C_3-C_7-cycloalkyl, optionally substituted.

70. The compound according to Claim 68 wherein the hydrophobic region feature is selected from an optionally substituted phenyl.

71. The compound according to Claim 68 wherein the compound has a binding affinity for KSP of about 0.1nM to about 100nM.

72. The compound according to Claim 68 wherein the compound does not comprise a 2-thioxo-1,2,3,4-tetrahydopyrimidine moiety, a dihydropyrimidine moiety or a 5,6,11,11a-tetrahydro-1H-imidazo[1',5':1,6]-pyrido[3.4-b]indole-1,3(2H)-dione moiety.

73. A compound, comprising three hydrophobic region features and a hydrogen bond acceptor feature, wherein said features are spatially oriented as illustrated in Figure 16 and have the distances in Å between the features as follows

	1	2	3	4
1	-			
2	5.1±0.6	-		
3	8.5±0.7	6.9±0.7	-	
4	3.7±0.5	5.8±0.6	5.7±0.7	-

and wherein said compound inhibits the mitotic kinesin KSP;
or a pharmaceutically acceptable salt thereof.

74. The compound according to Claim 73 wherein the compound does not comprise a quinazolinone, phenothiazine, thienopyrimidinone, furanopyrimidinone, azolopyrimidinone, thiazolopyrimidine, cycloalkylpyrimidinone or triphenylmethane moiety.

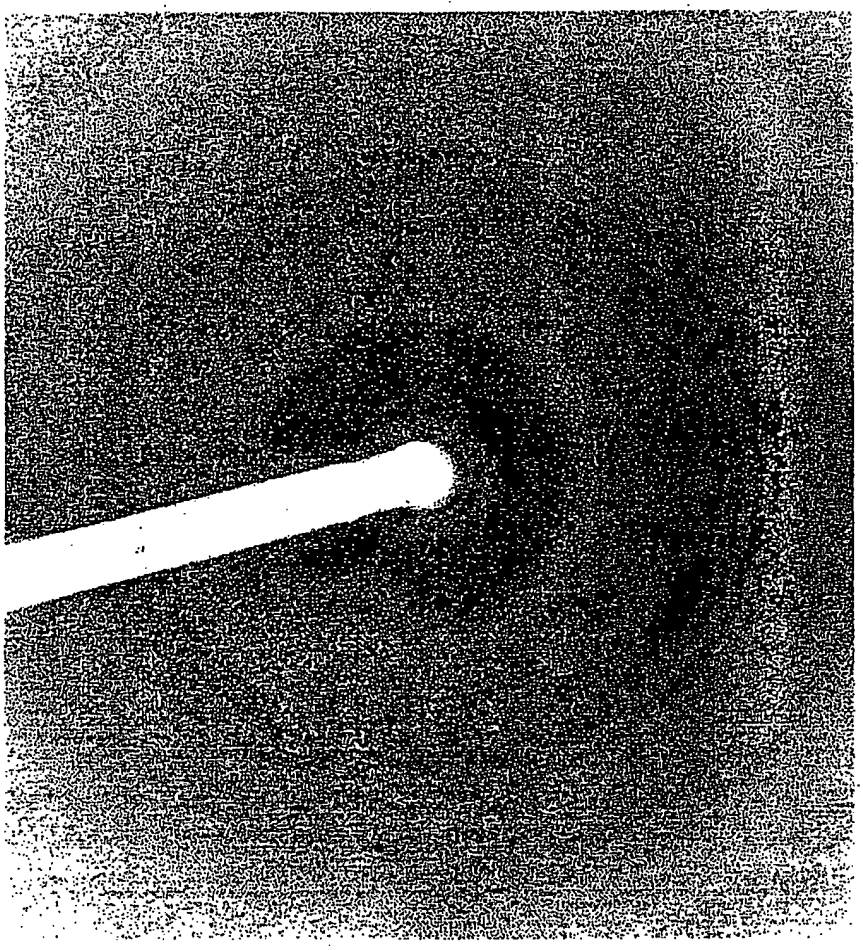


FIG. 1

BEST AVAILABLE COPY

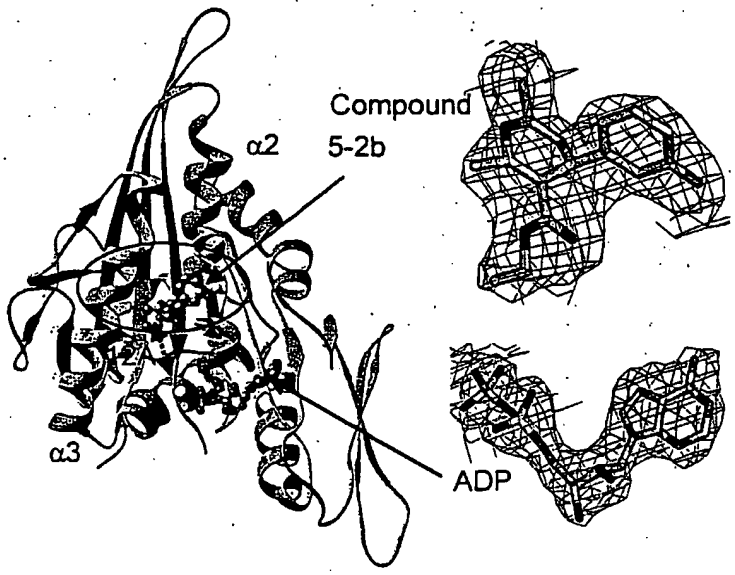


FIG.2

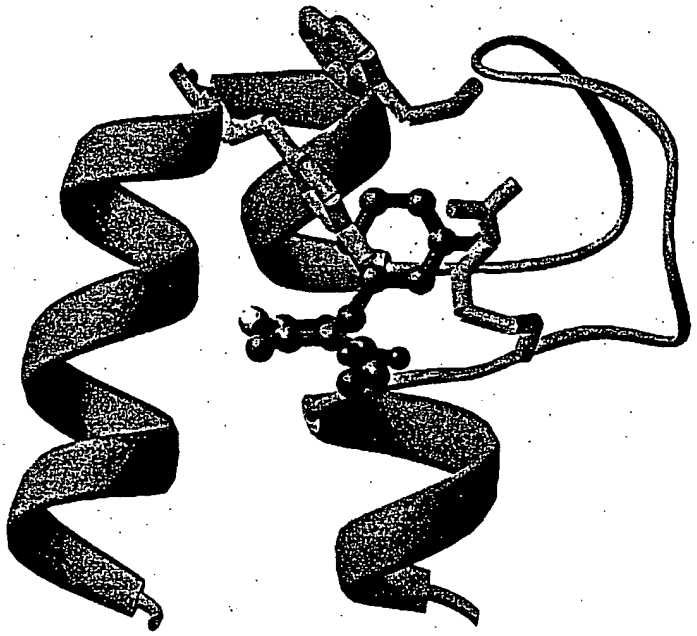


FIG.3

BEST AVAILABLE COPY

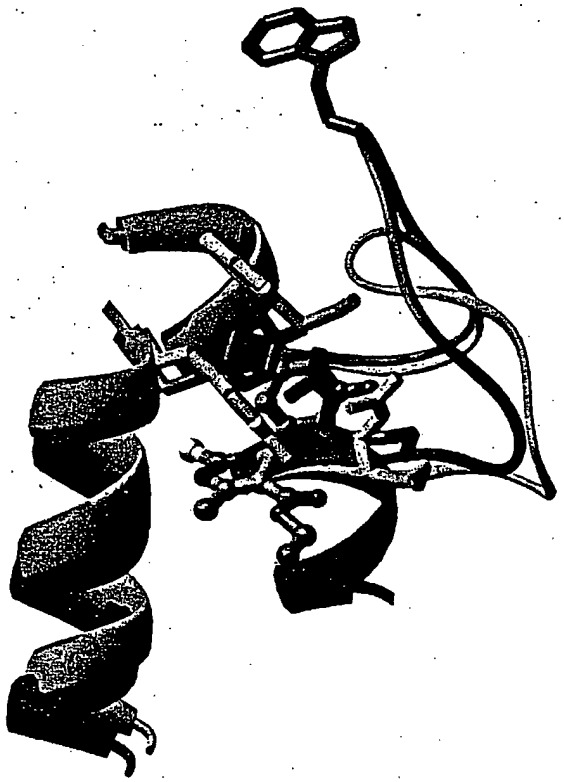


FIG.4

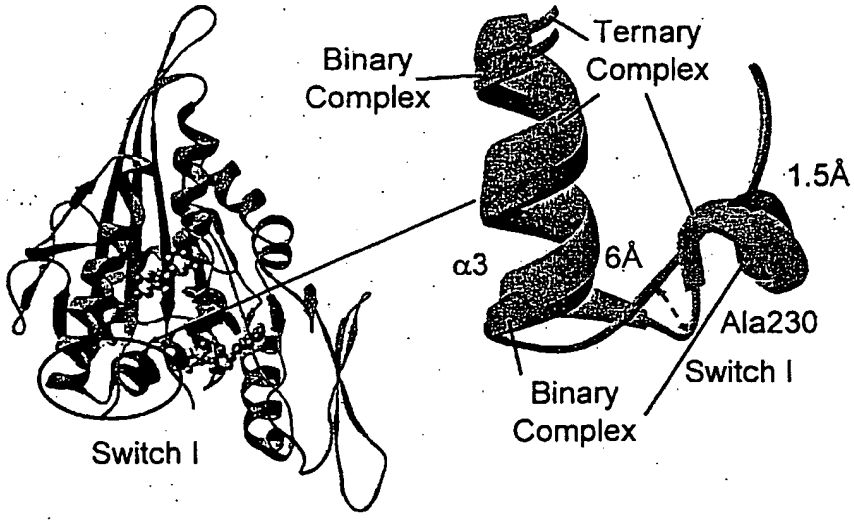

Binary
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Ternary
Complex
1.5Å
α3
6Å
Ala230
Switch I
Binary
Complex
Switch I

FIG.5

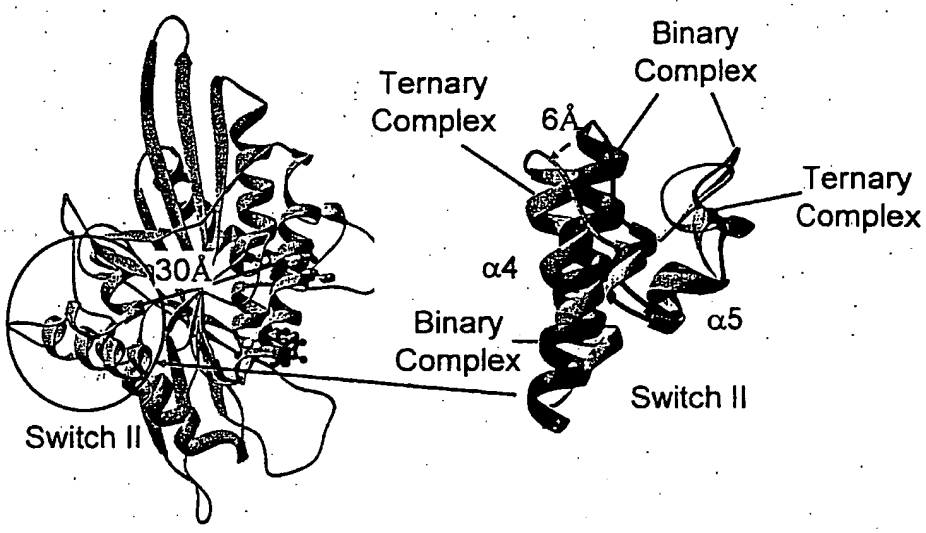

Binary
Complex
Ternary
Complex
6Å
Ternary
Complex
30Å
α4
α5
Binary
Complex
Switch II
Switch II

FIG.6

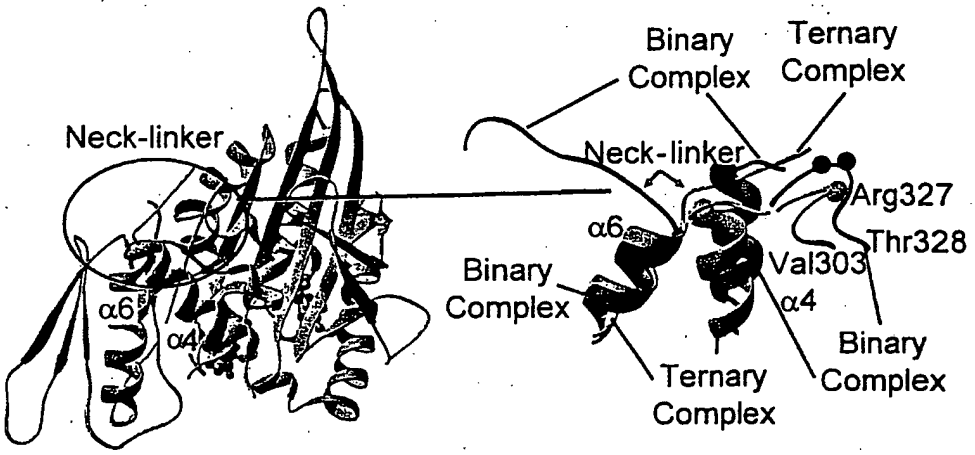

Neck-linker
α6
α4
Binary Complex
Ternary Complex
Neck-linker
α6
Binary Complex
Arg327
Thr328
Val303
α4
Binary Complex
Ternary Complex

FIG.7

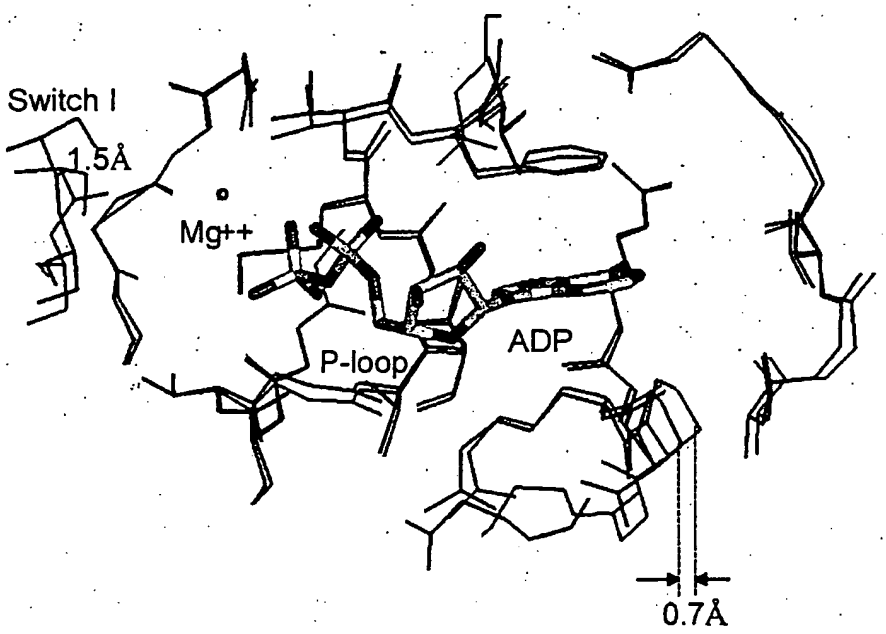


FIG.8

Seq. ID #1

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IFAYGQTGTG KTFTMEGERS PNEEYTWEED PLAGIIPRTL HQIFEKLTDN
GTEFSVKVSL LEIYNEELFD LLNPSSDVSE RLQMFDDPRN KRGVIIKGLE
EITVHNKDEV YQILEKGAAK RTTAATLMNA YSSRSHSVFS VTIHMKETTI
DGEELVKIGK LNLVDLAGSE NIGRSGAVDK RAREAGNINQ SLLTLGRVIT
ALVERTPHVP YRESKLTRIL QDSLGGRTRT SIIATISPAS LNLEETLSTL
EYAHRAKNIL NKPEVNQK

FIG.9

115(M), 116(E), 117(G), 118(E), 119(R);

127(W), 130(D), 132(L), 133(A), 134(G), 136(I), 137(P);

160(L); and

211(Y), 214(L), 215(E), 217(G), 218(A), 221(R), 239(F).

FIG.10

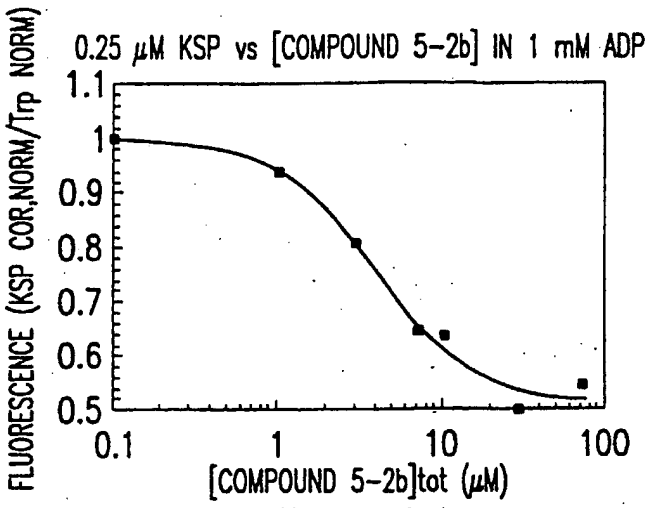


FIG.11A

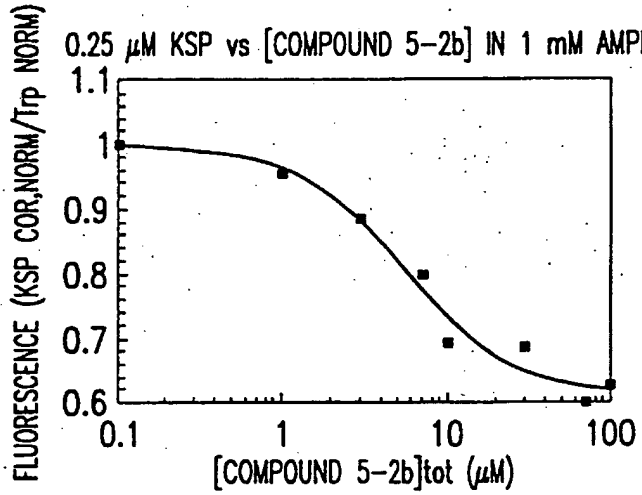


FIG.11B

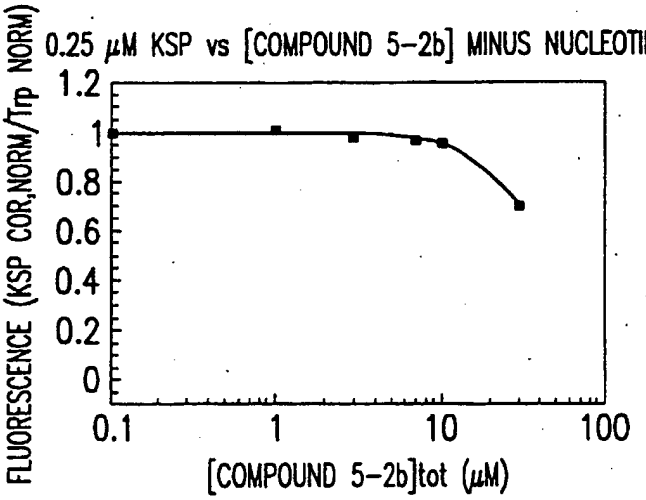


FIG.11C

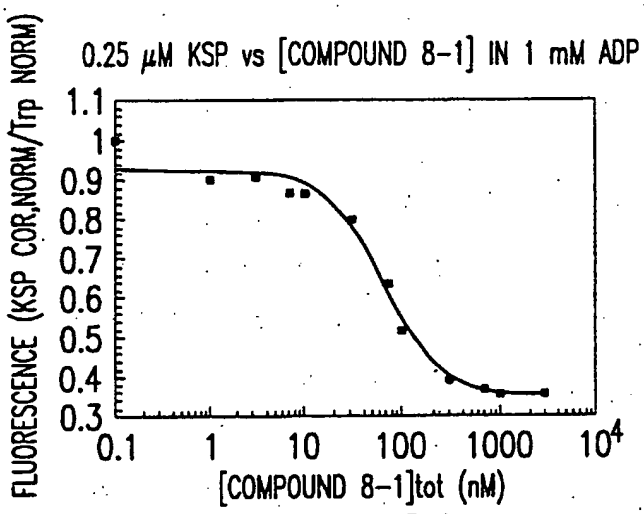


FIG.12A

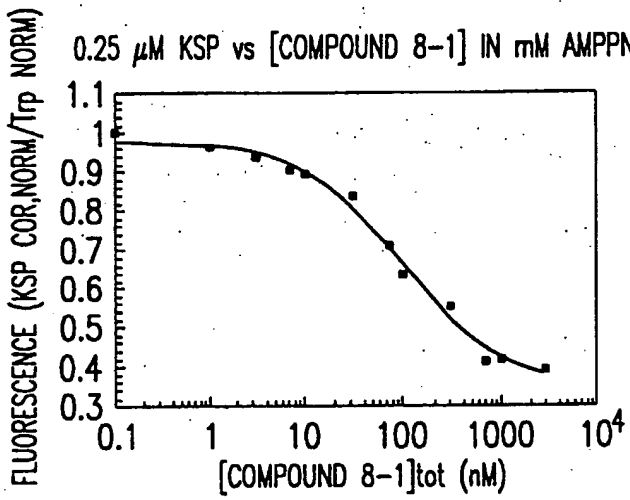


FIG.12B

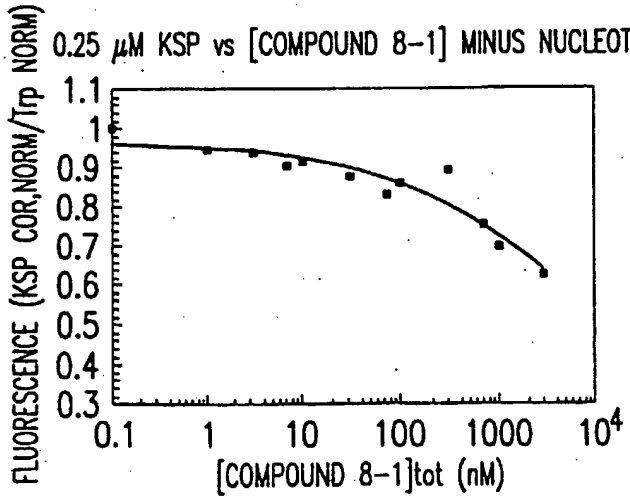


FIG.12C

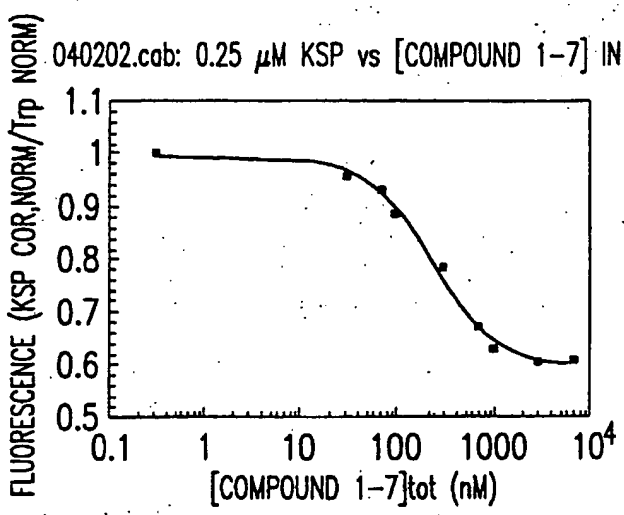


FIG.13A

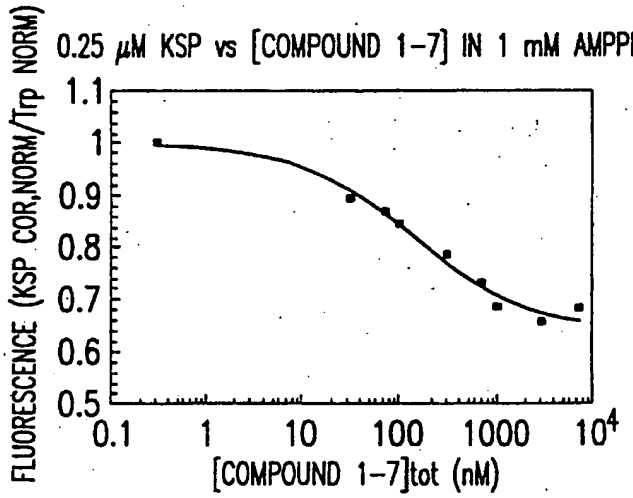


FIG.13B

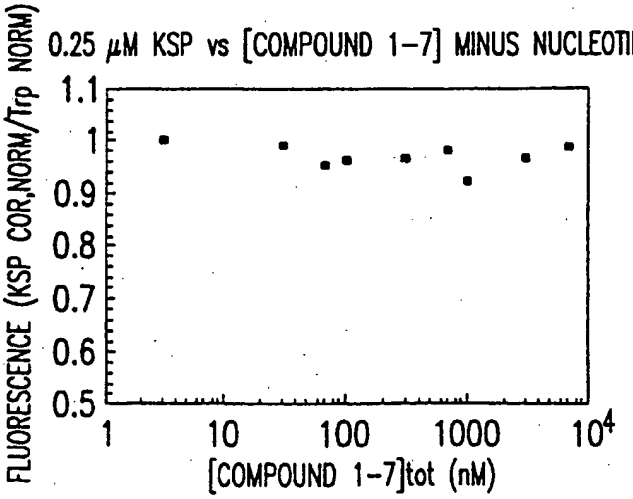


FIG.13C

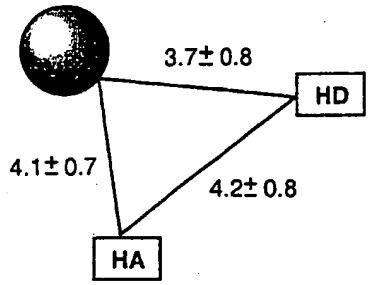


FIG. 14A

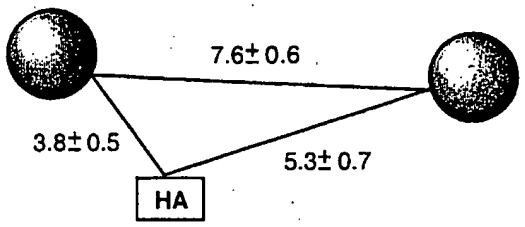


FIG. 14B

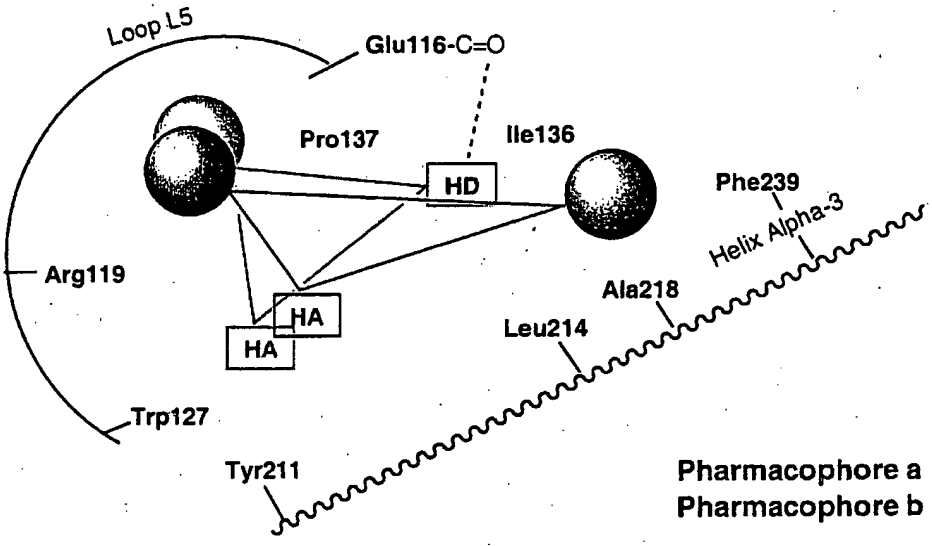

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HD
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Helix Alpha-3
Arg119
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HA
HA
Leu214
Trp127
Tyr211
Pharmacophore a
Pharmacophore b

FIG. 15

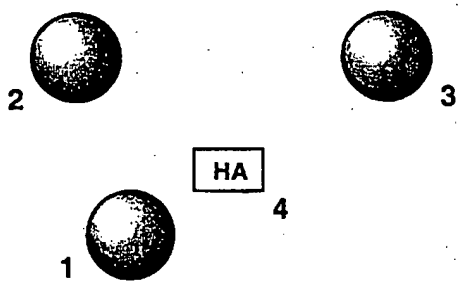


FIG. 16

SEQUENCE LISTING

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Buser-Doepner, Carolyn A.
Coleman, Paul J.
Cox, Christopher D.
Fraley, Mark E.
Garbaccio, Robert M.
Hartman, George D.
Heimbrook, David C.
Huber, Hans E.
Kuo, Lawrence C.
Sardana, Vinod V.
Torrent, Maricel
Youwei, Yan

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Arg Lys Ala Ser Ala His Ser Ile Val Glu Cys Asp Pro Val Arg Lys
        35                  40                  45
Glu Val Ser Val Arg Thr Gly Gly Leu Ala Asp Lys Ser Ser Arg Lys
    50                  55                  60
Thr Tyr Thr Phe Asp Met Val Phe Gly Ala Ser Thr Lys Gln Ile Asp
65                  70                  75                  80
Val Tyr Arg Ser Val Val Cys Pro Ile Leu Asp Glu Val Ile Met Gly
                85                  90                  95
Tyr Asn Cys Thr Ile Phe Ala Tyr Gly Gln Thr Gly Thr Gly Lys Thr
            100                 105                 110
Phe Thr Met Glu Gly Glu Arg Ser Pro Asn Glu Glu Tyr Thr Trp Glu
        115                 120                 125
Glu Asp Pro Leu Ala Gly Ile Ile Pro Arg Thr Leu His Gln Ile Phe
    130                 135                 140
Glu Lys Leu Thr Asp Asn Gly Thr Glu Phe Ser Val Lys Val Ser Leu
145                 150                 155                 160
Leu Glu Ile Tyr Asn Glu Glu Leu Phe Asp Leu Leu Asn Pro Ser Ser
                165                 170                 175
Asp Val Ser Glu Arg Leu Gln Met Phe Asp Asp Pro Arg Asn Lys Arg
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Ala Thr Leu Met Asn Ala Tyr Ser Ser Arg Ser His Ser Val Phe Ser
225                 230                 235                 240
Val Thr Ile His Met Lys Glu Thr Thr Ile Asp Gly Glu Glu Leu Val
                245                 250                 255
Lys Ile Gly Lys Leu Asn Leu Val Asp Leu Ala Gly Ser Glu Asn Ile
            260                 265                 270
Gly Arg Ser Gly Ala Val Asp Lys Arg Ala Arg Glu Ala Gly Asn Ile
        275                 280                 285
Asn Gln Ser Leu Leu Thr Leu Gly Arg Val Ile Thr Ala Leu Val Glu
    290                 295                 300
Arg Thr Pro His Val Pro Tyr Arg Glu Ser Lys Leu Thr Arg Ile Leu
305                 310                 315                 320
Gln Asp Ser Leu Gly Gly Arg Thr Arg Thr Ser Ile Ile Ala Thr Ile
                325                 330                 335
Ser Pro Ala Ser Leu Asn Leu Glu Glu Thr Leu Ser Thr Leu Glu Tyr
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